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A Feynman Path-Integral Calculation of the Polaron Effective Mass.

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A FEYNMAN PATH-INTEGRAL CALCULATION OF THE POLARON EFFECTIVE MASS

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ABSTRACT

In the expansion of the ground-state energy of a polaron in a weak magnetic field as a power series in the magnetic field strength, the zeroth-order term is the polaron self-energy while the first-order term is inversely proportional to the polaron effective mass. The effective mass so obtained is exactly equivalent to the free polaron effective mass as defined by Fröhlich. This equivalence principle is used to approximate the polaron effective mass by employing an approximate expression of the ground-state energy of a polaron in a weak magnetic field obtained by applying Feynman's path-integral variational method. The resultant polaron effective mass is found to be higher than Feynman's result by less than one per cent.

CONTENTS

CHAPTER I

INTRODUCTION

The polaron problem arises in the study of the motion of a single electron in the conduction band of a semiconductive ionic crystal. The usual initial approach to the description of a conduction electron is the Bloch approximation[1] which assumes that the lattice ions are rigidly attached to their lattice sites. In the Bloch approximation an electron with energy near the bottom of the conduction band moves as a free particle with a certain mass m, called the band mass. For an ionic crystal this approximation is an over simplification because in such crystals the lattice ions are unshielded charges and therefore react significantly to the presence of a conduction electron. Thus the conduction electron induces an appreciable displacement of the lattice ions from the static configuration assumed in the Bloch approximation. The electron in turn experiences not only the static field assumed in the Bloch approximation but also the incremental electric field resulting from the displacement of the lattice ions from their lattice sites. If one assumes that the wave vector of electron is small compared to the reciprocal lattice spacing (which is tantamount to saying that electronic wave function will vary only negligibly over the distance of several lattice spacings) then the electron can be regarded essentially as moving under the

influence of a continuous macroscopic polarization field arising from the displacement of ions from their lattice sites. The name "polaron" has been given to the entity consisting of the Bloch conduction electron together with its accompanying (non-radiative) polarization field. Another way to look at the motion of electron in an ionic crystal is to regard the electron as triggering quantized vibrations (phonons) in the crystal. Then the polaron is the Bloch electron "dressed" with its cloud of phonons.

In a derivation[2] of the Hamiltonian for such a system, Fröhlich invokes the additional approximation that the electron interacts predominantly with long wavelength longitudinal optical (LO) modes of the crystal all of which are treated as having a common frequency, ω. Fröhlich's Hamiltonian is derived in Appendix A and is given by*

$$H(\alpha) = \frac{1}{2}\,\underset{\sim}{p}^2 + \sum_{\underset{\sim}{k}} \frac{1}{2}\,(p_{\underset{\sim}{k}}^2 + q_{\underset{\sim}{k}}^2 - 1) + \left[\frac{8\sqrt{2}\pi\alpha}{V}\right]^{\frac{1}{2}} \sum_{\underset{\sim}{k}} \frac{1}{|\underset{\sim}{k}|}\, q_{\underset{\sim}{k}} \begin{Bmatrix} \cos \underset{\sim}{k}\cdot\underset{\sim}{r} \\ \sin \underset{\sim}{k}\cdot\underset{\sim}{r} \end{Bmatrix}, \qquad (1)$$

where $\underset{\sim}{r}$ is the electron coordinate vector, $q_{\underset{\sim}{k}}$ is the polarization-field oscillator coordinate of wave vector $\underset{\sim}{k}$, $\underset{\sim}{p}$ and $p_{\underset{\sim}{k}}$ are the momenta canonically conjugate to $\underset{\sim}{r}$ and $q_{\underset{\sim}{k}}$, and α is a dimensional constant called the polaron

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* Throughout this paper a natural system of units is used in which $m=\omega=\hbar=1$.

coupling constant defined by

$$\alpha = \frac{1}{2}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon}\right)\frac{e^2}{\hbar\omega}\left(\frac{2m\omega}{\hbar}\right)^{\frac{1}{2}}, \tag{2}$$

wherein $-e$ is the electronic charge and ε and ε_∞ are the static and optical dielectric constants of crystal. In Eq. (1) V is a normalization volume which is to be taken infinitely large, in which limit

$$\sum_{\underset{\sim}{k}} \rightarrow \frac{V}{8\pi^3}\int d^3\underset{\sim}{k}. \tag{3}$$

The notation

$$\left\{\begin{matrix}\cos \underset{\sim}{k}\cdot\underset{\sim}{r} \\ \sin \underset{\sim}{k}\cdot\underset{\sim}{r}\end{matrix}\right\} \tag{4}$$

stands for the upper or the lower expression depending respectively on whether or not $\underset{\sim}{k}$ satisfies one or the other of the following:

$$k_x > 0,$$

$$k_x = 0,\ k_y > 0,$$

or

$$k_x = 0,\ k_y = 0,\ k_z > 0. \tag{5}$$

The first term in the Hamiltonian given by Eq. (1) is the band energy of the electron measured from the bottom of the conduction band, the second term represents the energy of the polarization field measured relative to its zero-point energy, and the third term is the electron-LO-phonon interaction energy.

Fröhlich[2] also defines the polaron self-energy, $E_o(\alpha)$, and the polaron effective mass, $\mu(\alpha)$, by the expansion

$$E_o(\alpha,\underset{\sim}{k}_T) = E_o(\alpha) + \frac{1}{2\mu(\alpha)}\,\underset{\sim}{k}_T^2 + O(\underset{\sim}{k}_T^4), \tag{6}$$

where $E_o(\alpha,\underset{\sim}{k}_T)$ is the ground-state eigenvalue of $H(\alpha)$, whose corresponding eigenfunction, $\psi_{o,\underset{\sim}{k}_T}$, is also an eigenfunction of the total wave vector, $\underset{\sim}{K}_T$, with eigenvalue $\underset{\sim}{k}_T$. The total wave vector, $\underset{\sim}{K}_T$, means the vector sum of the wave vectors of the electron and all the phonons. By definition, $\psi_{o,\underset{\sim}{k}_T}$ depicts a situation in which all phonons present are non-radiative and are therefore part of the polaron's phonon cloud. Thus $E_o(\alpha,\underset{\sim}{k}_T)$ represents the energy of a ground-state polaron propagating with a wave vector $\underset{\sim}{k}_T$.

The polaron problem has been of long standing interest in physics. From a theoretical viewpoint it is of interest because it affords a relatively simple but non trivial example of an interaction between a particle

and its self-produced quantized field in which no troublesome infinite renormalizations arise. Because of this extended interest, the coupling constant, α, is regarded as an independent parameter. One of the aims of the theoretical research is to develop calculational methods which are accurate for all values of the coupling constant, α, with the hope that such methods may be helpful in dealing with similar many-body problems such as a nucleon interacting with its meson field.

Recent experimental investigations on polarons have further stimulated the theoretical work on the subject. First, the experiments on the ionization energy of bound polarons,[3,4] require for their interpretation the theoretical difference in energy of the free-polaron ground-state energy and the energy of the bound polarons. Since these energies are usually calculated separately, it is important to have good values for the free-polaron ground-state energy. Second, polaron effective masses have been estimated experimentally by cyclotron resonance measurements made on a variety of materials in which the polaron coupling constant, α, lies in the range $1<\alpha<4.5$.[5-8] It would be desirable, therefore, to have a reasonably accurate formula for the polaron effective mass as a function of the polaron coupling constant (which in turn is known in terms of the band mass by Eq. (2)) because such a formula can be used in conjunction with the

experimentally determined polaron mass to compute the band mass for the sake of comparison with independent theoretical calculations for the band mass.

Various theoretical methods[9,10] have been employed to approximate the polaron self-energy and effective mass. The Lee-Low-Pines[11] weak-coupling variational calculation yields

$$E_o = -\alpha \ , \tag{7}$$

and

$$\mu(\alpha) = 1 + \frac{1}{6}\alpha \ . \tag{8}$$

These results are exactly correct to the first order in α in the limit of weak coupling. Several more refined weak-coupling theories have been published.[9,12,13,14]

The strong-coupling variational calculations of Landau[15] and Pekar[16] yield

$$E_o(\alpha) = -a\alpha^2 \ , \tag{9}$$

and

$$\mu'(\alpha) = b\alpha^4 + 1 \ , \tag{10}$$

with

$$a \simeq .10 \ , \tag{11}$$

and

$$b \simeq .02 \ . \tag{12}$$

The analytic form of Eq. (9) is asymptotically correct.[17] The polaron effective mass, $\mu'(\alpha)$, given by Eq. (10), however, is based upon an alternative definition of the effective mass which is equivalent to Fröhlich's definition only when the trial ground-state wave function employed is an exact eigenfunction of the total wave vector. The trial wave function employed in Landau-Pekar approximation is not such a function. A few further refinements in the strong-coupling theories have also been worked out.[9,18]

The Feynman-Schultz[19,20] results for the polaron self-energy and effective mass agree with the Lee-Low-Pines result for weak coupling, agree with the Landau-Pekar results for strong coupling and possess smooth transitional behavior for intermediate coupling. For all values of α, the self-energy obtained by Feynman and Schultz is an upper-bound approximation which is less than or approximately equal to all other known upper bounds to the

self-energy. Therefore the Feynman-Schultz method is remarkably successful at least for the purpose of calculating the ground-state energy of a free polaron for all coupling strengths. Their polaron effective mass, however, is based on a definition which (although ingeniously devised for ease of calculation within the framework of their method of approximation) is rather ad hoc in the respect that no rigorous validation is offered for equating the result to the "true" polaron effective mass as already properly defined by Fröhlich.

In this paper the ground-state energy of a polaron in a weak magnetic field, $\underset{\sim}{B}$, will be calculated using the same variational approximation as Feynman and Schultz used to calculate the ground-state energy of a free polaron. In view of their success in the free polaron case, it is expected that the results for a weak magnetic field would be accurate at least to first order in the magnetic field strength. Once the ground-state energy of a polaron in a weak magnetic field is calculated to first order in the magnetic field strength, then a corresponding approximation for the free polaron effective mass can be obtained by invoking a theorem (proved by Marshall and Robert[21] and shown in Appendix B) according to which

$$E_o(\alpha,\lambda) = E_o(\alpha) + \frac{1}{2}\frac{\lambda}{\mu(\alpha)} + O(\lambda^2), \tag{13}$$

where

$$\lambda = eB/c, \tag{14}$$

where $E_o(\alpha,\lambda)$ is the exact ground-state energy of a polaron in a magnetic field, and where $E_o(\alpha)$ and $\mu(\alpha)$ are the exact self-energy and effective mass respectively of a free polaron as defined by Fröhlich.

The Feynman path-integral formulation for calculation of the exact ground-state energy of a polaron in a magnetic field is developed in Chapter 2. The variational approximation to the ground-state energy is carried out and the expression for the polaron effective mass is obtained in Chapter 3. The results are discussed in Chapter 4 along with comparisons with the results of Feynman and Schultz and the results of others, including those of Hellwarth and Platzman[22] who have obtained the polaron effective mass by a method somewhat similar to the present one.

CHAPTER 2

EXACT EXPRESSION FOR THE POLARON GROUND-STATE ENERGY

In order to derive an exact expression for the ground-state energy, $E_o(\alpha,\lambda)$, of a polaron in a magnetic field, one may begin by noting that if the polaron system is in any specified state, Ψ, at an initial time ($t=0$), then the system's wave function at any later time ($t=t_f$), is expressible as

$$\Psi(\underset{\sim}{r}_f,q_f,t_f) = \int d^3\underset{\sim}{r}_i \int dq_i K(\underset{\sim}{r}_f,q_f,t_f;\underset{\sim}{r}_i,q_i 0)\Psi(\underset{\sim}{r}_i,q_i,0), \tag{15}$$

where $q \equiv \{q_{\underset{\sim}{k}}\}$ represents the set of all polarization field oscillators and

$$K(\underset{\sim}{r}_f,q_f,t_f;\underset{\sim}{r}_i,q_i,0) \equiv \sum_n \psi_n(\underset{\sim}{r}_f,q_f)\psi_n^*(\underset{\sim}{r}_i,q_i)e^{-iE_n(\alpha,\lambda)t_f}, \tag{16}$$

wherein $\psi_n(\underset{\sim}{r},q)$ represents a complete orthonormal set of eigenfunctions of the Hamiltonian, $H(\alpha,\lambda)$, of a polaron in a magnetic field and $E_n(\alpha,\lambda)$ represents the corresponding energy eigenvalues. Equation (16) may be solved for the ground-state energy, $E_o(\alpha,\lambda)$, in the following

convenient way:

Let $\phi_o(q)$ be any function of q which is not orthogonal to the exact ground state function $\psi_o(\underset{\sim}{r},q)$. Multiplication of both sides of Eq. (16) by $\phi_o(q_i)\cdot\phi_o^*(q_f)$ and integration over the variables q_f and q_i gives

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dq_f\, dq_i\, \phi_o^*(q_f)K(\underset{\sim}{r}_f,q_f,t_f;\underset{\sim}{r}_i,q_i,o)\phi_o(q_i) =$$

$$\sum_n a_{no}(\underset{\sim}{r}_f)\, a_{no}^*(\underset{\sim}{r}_i)e^{-iE_n(\alpha,\lambda)t_f}, \tag{17}$$

where

$$a_{no}(\underset{\sim}{r}) = \int dq\, \phi_o^*(q)\psi_n(\underset{\sim}{r},q). \tag{18}$$

Evaluation of this result at $\underset{\sim}{r}_i = \underset{\sim}{r}_f = \underset{\sim}{0}$ and $t_f = -iT$, with $T \to +\infty$ yields

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dq_f\, dq_i\, \phi_o^*(q_f)K(\underset{\sim}{0},q_f,-iT;\underset{\sim}{0},q_i,0)\phi_o(q_i)$$

$$= \sum_n a_{no}(\underset{\sim}{0})\, a_{no}^*(\underset{\sim}{0})e^{-E_n(\alpha,\lambda)T} \tag{19}$$

$$\to a_{oo}(\underset{\sim}{0})\, a_{oo}^*(\underset{\sim}{0})e^{-E_o(\alpha,\lambda)T}. \tag{20}$$

Therefore

$$E_o(\alpha,\lambda) = \lim_{T\to\infty} \{-T^{-1} \ln G_{oo}(-iT)\}, \tag{21}$$

where

$$G_{oo}(t_f) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dq_f\, dq_i\, \phi_o^*(q_f) K(0,q_f,t_f;0,q_i,t_i)\phi_o(q_i). \tag{22}$$

Equation (21) along with Eq. (22) gives an exact expression for the polaron ground-state energy in terms of the kernel, K, which may be expressed explicitly as[23]

$$K(\underset{\sim}{r}_f,q_f,t_f;\underset{\sim}{r}_i,q_i,0) = \int_{\underset{\sim}{r}_{i,o}}^{\underset{\sim}{r}_f,t_f} D\underset{\sim}{r}(t) \int_{q_{i,o}}^{q_f,t_f} Dq(t) e^{iS}, \tag{23}$$

where

$$S = \int_o^{t_f} dt\, L(\underset{\sim}{r},\dot{\underset{\sim}{r}},q,\dot{q},\lambda) \tag{24}$$

and where L is the polaron Lagrangian in the presence of the magnetic field, $\underset{\sim}{B}$. This Lagrangian is derived in Appendix A in the form

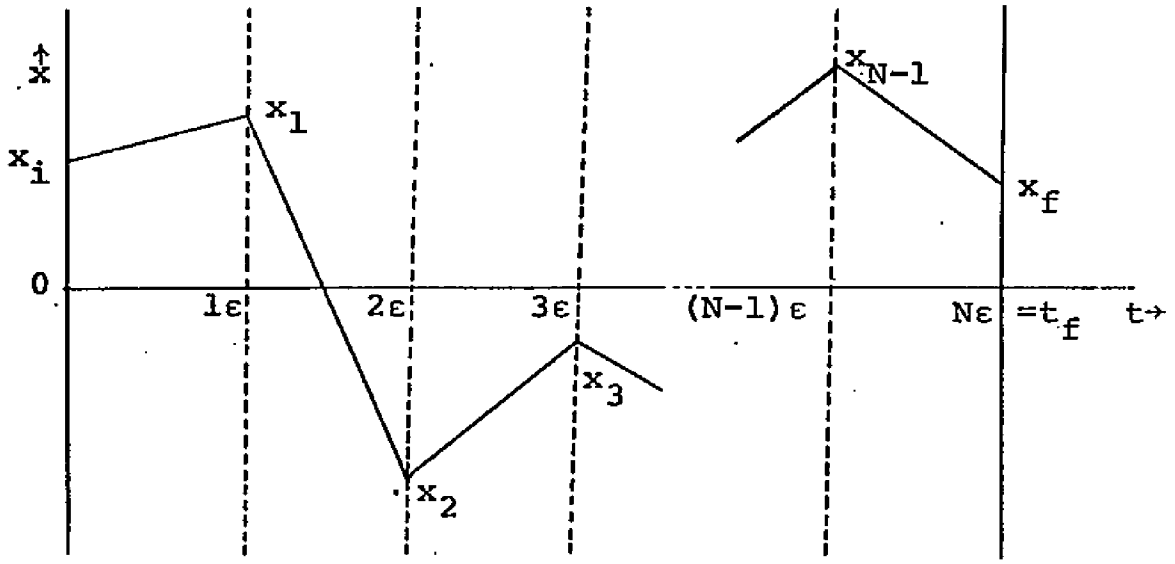
$$L(\underset{\sim}{r},\dot{\underset{\sim}{r}},q,\dot{q},\lambda) = \frac{1}{2}\,\dot{\underset{\sim}{r}}^2 + \lambda\dot{x}y + \frac{1}{2}\sum_{\underset{\sim}{k}}(\dot{q}_{\underset{\sim}{k}}^2-\dot{q}_{\underset{\sim}{k}}^2+1)$$

$$- \left[\frac{8\sqrt{2}\pi\alpha}{V}\right]^{\frac{1}{2}} \sum_{\underset{\sim}{k}} \frac{q_{\underset{\sim}{k}}}{|\underset{\sim}{k}|} \begin{Bmatrix} \cos \underset{\sim}{k}\cdot\underset{\sim}{r} \\ \sin \underset{\sim}{k}\cdot\underset{\sim}{r} \end{Bmatrix}. \qquad (25)$$

The notation

$$\int_{x_{i,o}}^{x_f,t_f} F[x(t)]Dx(t) \qquad (26)$$

denotes a single-fold Feynman path integral over paths, $x(t)$, satisfying the boundary conditions $x(o)=x_i$ and $x(t_f)=x_f$. This Feynman path integral is defined by the following set of operations: The interval $[o,t_f]$ is divided N subintervals, each of length $\varepsilon=t_f/N$.



Then

$$\int_{x_i,o}^{x_f,t_f} Dx(t)F[x(t)] = \lim_{N\to\infty}\left[\frac{N}{2\pi i t_f}\right]^{N/2} \cdot \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \int_{-\infty}^{\infty} dx_{N-1} F[x(t)], \tag{27}$$

where

$$x(t) = \begin{cases} x_i + \dfrac{x_1 - x_i}{\varepsilon}[t-o] & \text{for } o \le t \le 1\varepsilon \\ x_1 + \dfrac{x_2 - x_1}{\varepsilon}[t-\varepsilon] & \text{for } 1\varepsilon \le t \le 2\varepsilon \\ \vdots & \\ x_{N-1} + \dfrac{x_F - x_{N-1}}{\varepsilon}[t-(N-1)\varepsilon] & \text{for } (N-1)\varepsilon \le t \le N\varepsilon. \end{cases} \tag{28}$$

In Eq. (23), the symbol, $D\underset{\sim}{r}(t)$, denotes path integration over each of the three rectangular components of $\underset{\sim}{r}$, and $Dq(t)$, denotes the path integration over all oscillator coordinates, the integration over each coordinate being performed in the manner just indicated.

The fact that Eq. (23) does represent the kernel given by Eq. (16) can be verified by demonstrating that

it satisfies the following two conditions which are clearly true in view of Eq. (16) and which are sufficient to determine $K(\underset{\sim}{r}_f,q_f,t_f;\underset{\sim}{r}_i,q_i,o)$ uniquely:

$$\lim_{t_f\to\infty} K(\underset{\sim}{r}_f,q_f,t_f;\underset{\sim}{r}_i,q_i,o) = \delta(\underset{\sim}{r}_f-\underset{\sim}{r}_i)\delta(q_f-q_i), \tag{29}$$

and

$$H_f(\alpha,\lambda)K(\underset{\sim}{r}_f,q_f,t_f;\underset{\sim}{r}_i,q_i,o) = i\frac{\partial}{\partial t_f} K(\underset{\sim}{r}_f,q_f,t_f;\underset{\sim}{r}_i,q_i,o), \tag{30}$$

where the subscript "f" on $H(\alpha,\lambda)$ indicates operation on functions of f-subscripted coordinates and $H(\alpha,\lambda)$ denotes the Hamiltonian for a polaron in a magnetic field, derived in Appendix A and given there by Eq. (A66).

Equations (21)-(28) now constitute an exact explicit prescription for obtaining the ground-state energy, $E_o(\alpha,\lambda)$. To simplify this result, Eq. (22) may be written in the following more compact form

$$G_{oo}(t_f) = \int_{\underset{\sim}{o},o}^{\underset{\sim}{o},t_f} D\underset{\sim}{r}(t)\exp\{i\int_o^{t_f} dt(\tfrac{1}{2}\dot{\underset{\sim}{r}}^2 + \lambda\dot{x}y)\} \prod_{\underset{\sim}{k}} G_{\underset{\sim}{k}}(t_f), \tag{31}$$

where

$$G_{\underset{\sim}{k}}(t_f) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dq_{\underset{\sim}{k},f}\, dq_{\underset{\sim}{k},i}\, \phi_o^*(q_{\underset{\sim}{k},f}) \cdot \int_{q_{\underset{\sim}{k},i,o}}^{q_{\underset{\sim}{k},f},t_f} Dq_{\underset{\sim}{k}}(t) \exp\{i\int_o^{t_f} L_{\underset{\sim}{k}}(t)\,dt\}\phi_o(q_{\underset{\sim}{k},i}), \tag{32}$$

with

$$L_{\underset{\sim}{k}}(t) = \tfrac{1}{2}\,[\dot{q}_{\underset{\sim}{k}}^2 - q_{\underset{\sim}{k}}^2 + 1] - \gamma_{\underset{\sim}{k}}(t) q_{\underset{\sim}{k}}(t), \tag{33}$$

in which

$$\gamma_{\underset{\sim}{k}}(t) = \left[\frac{8\sqrt{2}\pi\alpha}{V}\right]^{\frac{1}{2}} \frac{1}{|\underset{\sim}{k}|} \begin{Bmatrix} \cos \underset{\sim}{k}\cdot\underset{\sim}{r} \\ \sin \underset{\sim}{k}\cdot\underset{\sim}{r} \end{Bmatrix}. \tag{34}$$

By choosing $\phi_o(q_{\underset{\sim}{k}})$ to be the simple harmonic oscillator ground-state function

$$\phi_o(q_{\underset{\sim}{k}}) = \pi^{-\frac{1}{4}} \exp\left(-\tfrac{1}{2} q_{\underset{\sim}{k}}^2\right), \tag{35}$$

each of the ordinary single integrals which result from using Definition (27) in Eq. (32) has an integrand of the simple form of an exponential of a quadratic function of its integration variable. Therefore, each such integral can be performed analytically. The result is[24]

$$G_{\underset{\sim}{k}}(t_f) = \exp\{ -\frac{1}{4} \int_o^{t_f} \int_o^{t_f} dt\, ds\, \gamma_{\underset{\sim}{k}}(t)\gamma_{\underset{\sim}{k}}(s) e^{-i|t-s|} \}. \tag{36}$$

The simplicity of this result is the motivation of the choice of ϕ_o as given by Eq. (35).

Substitution of Eq. (36) into Eq. (31) yields

$$G_{oo}(t_f) = \int_{\underset{\sim}{o},o}^{\underset{\sim}{o},t_f} D\underset{\sim}{r}(t)\, \exp\{ i \int_o^{t_f} dt \left(\frac{1}{2}\, \dot{\underset{\sim}{r}}^2 + \lambda \dot{x} y\right) - \frac{1}{4} \int_o^{t_f} \int_o^{t_f} dt\, ds\, e^{-i|t-s|} \sum_{\underset{\sim}{k}} \gamma_{\underset{\sim}{k}}(t)\gamma_{\underset{\sim}{k}}(s) \}. \tag{37}$$

The summation occuring in Eq. (37) can be evaluated by use of Eqs. (3) and (34) with the result that

$$\sum_{\underset{\sim}{k}} \gamma_{\underset{\sim}{k}}(t)\gamma_k(s) = \frac{\sqrt{2}\alpha}{|\underset{\sim}{r}(t) - \underset{\sim}{r}(s)|}\,. \tag{38}$$

Substitution of Eq. (38) into Eq. (37) and evaluation of the resulting equation for $t_f = -iT$ yields (upon making the simple change of variables of integration, $t \to -it$, $s \to -is$)

$$G_{oo}(-iT) = \int_{\underset{\sim}{o},o}^{\underset{\sim}{o},T} D\underset{\sim}{r}(t)e^{S}, \tag{39}$$

where

$$S = \int_{o}^{T} dt\left(-\frac{1}{2}\dot{\underset{\sim}{r}}^{2} + i\lambda\dot{x}y\right)$$

$$+ \frac{\alpha}{\sqrt{8}} \int_{o}^{T}\int_{o}^{T} dt\, ds\, \frac{e^{-|t-s|}}{|\underset{\sim}{r}(t)-\underset{\sim}{r}(s)|}, \tag{40}$$

and where the path integral in Eq. (39) (as well as each path integral in the sequel) is redefined by replacing t_f by $-it_f$ in Eq. (27).

In summary the exact ground-state energy of a polaron in a magnetic field is given by

$$E_o(\alpha,\lambda) = \lim_{T\to\infty}\{-T^{-1}\ln\int_{\underset{\sim}{o},o}^{\underset{\sim}{o},T} D\underset{\sim}{r}(t)e^{S}\}, \tag{41}$$

wherein S is expressed by Eq. (40). This result is remarkable in that the original bona-fide many-body problem has been reduced to a one-body problem. In a formalism in which the electron can interact only locally with the polarization field, it is necessary to include a description of the field, with its infinitely many degrees of freedom, in order to keep track of the history of the dynamics of the electron. In the formalism of

Feynman path-integrals over entire electron trajectories, however, a given trajectory, $\underset{\sim}{r}(t)$, specifies a complete history of electron motion, so that no additional dynamical description is needed to specify the historical information already supplied by $\underset{\sim}{r}(t)$.

The reduced one-body problem has an interesting form which can be explicated by writing Eq. (40) in the form

$$S = -\int_0^T dt\, H(t), \tag{42}$$

where

$$H(t) = \frac{1}{2}\dot{\underset{\sim}{r}}^2 - i\lambda\dot{x}y - \frac{2\alpha}{\sqrt{8}}\int_0^t ds\, \frac{e^{-(t-s)}}{|\underset{\sim}{r}(t)-\underset{\sim}{r}(s)|}\,. \tag{43}$$

The integrand $H(t)$ of Eq. (42) formally may be regarded as a (complex) energy associated with the motion of the electron at a time t. The first term in the expression for $H(t)$ is the kinetic energy of the electron, the second term is the magnetic interaction term, and the last term is a potential energy of sorts. This potential energy has the form of an attractive coulombic interaction of the electron at time t with itself at an earlier time s. The exponential factor signifies that the self-interaction is stronger in the near past than it is in the distant past.

CHAPTER 3

In preceeding chapters a procedure for calculating the polaron ground-state energy and thereby obtaining the polaron effective mass has been outlined. However, it has not been possible to evaluate the path integral in Eq. (41). For a weak magnetic field, however, one may obtain a variational upper-bound approximation for $E_o(\alpha,\lambda)$ by use of an extension of Feynman's variational principle discussed in Appendix C. According to this principle, for a sufficiently weak magnetic field,

$$E_o(\alpha,\lambda) \leq E_o'(\alpha,\lambda), \tag{44}$$

where

$$E_o'(\alpha,\lambda) = E_o^{(o)}(\alpha,\lambda) - \lim_{T\to\infty} T^{-1} \langle S-S' \rangle, \tag{45}$$

wherein S is given by Eq. (40), S' represents any approximation to S, and

$$E_o^{(o)}(\alpha,\lambda) = \lim_{T\to\infty} \{-T^{-1} \ln \int_{\underset{\sim}{o},o}^{\underset{\sim}{o},T} D\underset{\sim}{r}(t) e^{S'}\} \tag{46}$$

is the ground-state energy in the approximation S = S'. The angle brackets in Eq. (45) denote the path average

defined by

$$\langle F[\underset{\sim}{r}(t)]\rangle = \frac{\int_{\underset{\sim}{o},o}^{\underset{\sim}{o},T} D\underset{\sim}{r}(t)\, F[\underset{\sim}{r}(t)]\, e^{S'}}{\int_{\underset{\sim}{o},o}^{\underset{\sim}{o},T} D\underset{\sim}{r}(t)\, e^{S'}}, \tag{47}$$

wherein $F[\underset{\sim}{r}(t)]$ represents any function of path.

In as much as S' is chosen to approximate S, $E_o'(\alpha,\lambda)$ as given by Eq. (45) represents a corresponding approximation to the ground-state energy $E_o(\alpha,\lambda)$ in the respects that $E_o'(\alpha,\lambda)$ is an expansion for $E_o(\alpha,\lambda)$ as a power series in (S-S') correct through first order in (S-S') and that the variational principle may be brought to bear in order to optimally determine any parameters contained in the choice for S'.

To employ the variational principle successfully one needs to select S' so that the path integrals involving S' in Eqs. (44)-(47) can be performed and that (apart from an irrelevant additive constant) S' does approximate S well at least for those paths, $\underset{\sim}{r}(t)$, which contribute significantly to $\int \exp(S)\, D\underset{\sim}{r}(t)$ and $\int \exp(S')\, D\underset{\sim}{r}(t)$. The expression for S' to be used here is chosen in the same way as Feynman chooses his S' for the case of a free polaron, that is, by replacing the attractive Coulombic

potential, $-\frac{\alpha}{\sqrt{8}} |\underset{\sim}{r}(t)-\underset{\sim}{r}(s)|^{-1} e^{-|t-s|}$ by a simple harmonic attractive potential $\frac{1}{2}C[\underset{\sim}{r}(t)-\underset{\sim}{r}(s)]^2 e^{-w|t-s|}$, where C and w are variational parameters. Thus

$$S' = \int_0^T dt[-\frac{1}{2}\dot{\underset{\sim}{r}}^2 + i\lambda\dot{x}y]$$

$$- \frac{1}{2} C \int_0^T\int_0^T dt\, ds\, e^{-w|t-s|}[\underset{\sim}{r}(t)-\underset{\sim}{r}(s)]^2. \qquad (48)$$

A refinement of choice for which the required path integrals can also be performed without much greater difficulty is[24]

$$S'_{ref} = \int_0^T dt[-\frac{1}{2}\dot{\underset{\sim}{r}}^2 + i\lambda\dot{x}y]$$

$$- \frac{1}{2}\int_0^T\int_0^T dt\, ds\, (\int_0^\infty dw' C(w') e^{-w'|t-s|})[\underset{\sim}{r}(t)-\underset{\sim}{r}(s)]^2,$$

(49)

where $C(w')$ is a variational function. Equation (49) reduces to Eq. (48) for the restriction

$$C(w') = C\delta(w'-w). \qquad (50)$$

This refinement, however, is not employed here because it is too difficult to carry it through to numerical fruition, mainly because of the complicated form of the integral equation for C(w') which results from optimization.

Substitution of Eqs. (40) and (48) into Eq. (45) and use of the Definition (47) yields

$$E_o'(\alpha,\lambda) = E_o^{(o)}(\alpha,\lambda) - (A+B), \tag{51}$$

where

$$A = \lim_{T\to\infty} \frac{\alpha}{\sqrt{8}T} \int_o^T \int_o^T d\tau\, d\sigma\, e^{-|\tau-\sigma|} \langle |\underset{\sim}{r}(\tau)-\underset{\sim}{r}(\sigma)|^{-1} \rangle, \tag{52}$$

and

$$B = \lim_{T\to\infty} \frac{1}{2} \frac{C}{T} \int_o^T d\tau\, d\sigma\, e^{-|\tau-\sigma|} \langle |\underset{\sim}{r}(\tau)-\underset{\sim}{r}(\sigma)|^{2} \rangle. \tag{53}$$

For the purpose of simplifying Eqs. (51)-(53), one may begin by expressing $|\underset{\sim}{r}(\tau)-\underset{\sim}{r}(\sigma)|^{-1}$ in terms of its Fourier transform as follows:

$$|\underset{\sim}{r}(\tau)-\underset{\sim}{r}(\sigma)|^{-1} = \int d^3\underset{\sim}{k}(2\pi^2k^2)^{-1} \exp\{i\underset{\sim}{k}\cdot[\underset{\sim}{r}(\tau)-\underset{\sim}{r}(\sigma)]\} \tag{54}$$

$$= \int d^3\underset{\sim}{k}(2\pi^2k^2)^{-1} \exp\{\int_o^T dt\ \underset{\sim}{f}(\underset{\sim}{k},t,\tau,\sigma)\cdot\underset{\sim}{r}(t)\}, \quad (55)$$

where

$$\underset{\sim}{f}(\underset{\sim}{k},t,\tau,\sigma) = i\underset{\sim}{k}[\delta(t-\tau) - \delta(t-\sigma)]. \quad (56)$$

Substitution of Eq. (55) into Eqs. (52) and (53) then yields

$$A = \lim_{T\to\infty} \frac{\alpha}{\sqrt{8}T} \int_o^T\int_o^T d\tau\ d\sigma\ e^{-|\tau-\sigma|}\int d^3\underset{\sim}{k}(2\pi^2k^2)^{-1}W(\underset{\sim}{k},\tau,\sigma) \quad (57)$$

and

$$B = \lim_{T\to\infty} \frac{1}{2}\frac{C}{T} \int_o^T\int_o^T d\tau\ d\sigma\ e^{-\omega|\tau-\sigma|}[-\nabla^2_{\underset{\sim}{k}}W(\underset{\sim}{k},\tau,\sigma)\Big|_{\underset{\sim}{k}=o}], \quad (58)$$

where

$$W(\underset{\sim}{k},\tau,\sigma) \equiv \langle\exp\{\int_o^T dt\ \underset{\sim}{f}(\underset{\sim}{k},t,\tau,\sigma)\cdot\underset{\sim}{r}(t)\}\rangle. \quad (59)$$

Furthermore, the evaluation of $E_o^{(o)}$, as given by Eq. (46), may be accomplished without direct use of the definition

of path integral by observing from Eqs. (46) and (48) that

$$C\left(\frac{\partial E_o^{(o)}(\alpha,\lambda,C,w)}{\partial C}\right)_{\alpha,\lambda,w} = B(C,w), \tag{60}$$

whereby

$$E_o^{(o)}(\alpha,\lambda) = \frac{\lambda}{2} + \int_o^C \frac{B(C,w)}{C}\, dC \tag{61}$$

because for C=0, S' describes the cyclotron motion of particle for which the ground-state energy is $\lambda/2$.

It is clear from Eqs. (51), (57), (58), and (61) that in order to obtain a tenable formula for $E_o'(\alpha,\lambda)$, a simplified expression is needed for $W(\underset{\sim}{k},\tau,\sigma)$ which by use of Eqs. (47) and (59) can be written explicitly as

$$W = \frac{\int_{\underset{\sim}{o},o}^{\underset{\sim}{o},T} D\underset{\sim}{r}(t)\exp\{[\int_o^T \underset{\sim}{f}(\underset{\sim}{k},t,\tau,\sigma)\cdot\underset{\sim}{r}(t)\,dt]+S'\}}{\int_{\underset{\sim}{o},o}^{\underset{\sim}{o},T} D\underset{\sim}{r}(t)\exp(S')}. \tag{62}$$

This expression may be simplified by changing the path-integration variable, $\underset{\sim}{r}(t)$, in the numerator of Eq. (62) to a new variable $\underset{\sim}{r}'(t) \equiv \underset{\sim}{r}(t) - \bar{\underset{\sim}{r}}(t)$, where $\bar{\underset{\sim}{r}}(t)$ is that path for which the exponent in the numerator of Eq. (62)

is extremal and for which $\underset{\sim}{r}(o) = \underset{\sim}{r}(T) = \underset{\sim}{0}$. The resultant numerator contains the denominator as a factor with the consequence that

$$W(\underset{\sim}{k},\tau,\sigma) = \exp\{\frac{1}{2}\int_o^T \underset{\sim}{f}(\underset{\sim}{k},t,\tau,\sigma)\cdot\bar{\underset{\sim}{r}}(t)dt\}. \tag{63}$$

Extremization of the exponent of the numerator of Eq. (62) yields the following integro-differential equations for the components of $\bar{\underset{\sim}{r}}(t)$:

$$\ddot{\bar{x}}(t) = 2C\int_o^T e^{-w|t-s|}[\bar{x}(t)-\bar{x}(s)]ds+i\lambda\dot{\bar{y}}-f_x(\underset{\sim}{k},t,\tau,\sigma), \tag{64}$$

$$\ddot{\bar{y}}(t) = 2C\int_o^T e^{-w|t-s|}[\bar{y}(t)-\bar{y}(s)]ds-i\lambda\dot{\bar{x}}-f_y(\underset{\sim}{k},t,\tau,\sigma), \tag{65}$$

and

$$\ddot{\bar{z}}(t) = 2C\int_o^T e^{-w|t-s|}[\bar{z}(t)-\bar{z}(s)]ds-f_z(\underset{\sim}{k},t,\tau,\sigma), \tag{66}$$

where f_x, f_y, and f_z are the components of $\underset{\sim}{f}$ given by Eq. (56). In Appendix D, these equations are solved conveniently in the limit $T\to\infty$, apart from additive constants which are irrelevant in view of Eqs. (56) and (63) and

apart from transient terms which are appreciable only near the end points t=o and t=T and which are also irrelevant to the desired evaluation of Eqs. (57) and (58) in the required limit $T\to\infty$. The results are

$$\bar{x}(t) = \int_o^T dt'\ G_{xx}(t,t') f_x(\underset{\sim}{k},t',\tau,\sigma) + \int_o^T dt'\ G_{xy}(t,t') f_y(\underset{\sim}{k},t',\tau,\sigma), \tag{67}$$

$$\bar{y}(t) = \int_o^T dt'\ G_{yy}(t,t') f_y(\underset{\sim}{k},t',\tau,\sigma) + \int_o^T dt'\ G_{yx}(t,t') f_x(\underset{\sim}{k},t',\tau,\sigma), \tag{68}$$

and

$$\bar{z}(t) = \int_o^T dt'\ G_{zz}(t,t') f_z(\underset{\sim}{k},t',\tau,\sigma), \tag{69}$$

where

$$G_{xy}(t,t') = -G_{yx}(t,t'), \tag{70}$$

$$G_{yy}(t,t') = G_{xx}(t,t'), \tag{71}$$

$$G_{xx}(t,t') = \bar{G}_{zz}(t,t') + \frac{1}{4}\lambda \frac{\ddot{w}^4}{v^4}(t-t')^2 + O(\lambda^2), \tag{72}$$

and

$$G_{zz}(t,t') = -\frac{1}{2v^2}\left[\frac{v^2-w^2}{v}\left(1-e^{-v|t-t'|}\right)+w^2|t-t'|\right], \tag{73}$$

wherein

$$v^2 \equiv w^2 + 4C/w. \tag{74}$$

Substitution of Eq. (56) and Eqs. (67)-(69) into Eq. (63) and use of Relations (70) and (71) yield

$$W(\underset{\sim}{k},\tau,\sigma) = \exp\{(k_x^2+k_y^2)G_{xx}(|\tau-\sigma|) + k_z^2 G_{zz}(|\tau-\sigma|)\}. \tag{75}$$

Equation (75) can be further simplified by substitution of G_{xx} in terms of G_{zz} from Eq. (72). The result is

$$W(\underset{\sim}{k},\tau,\sigma) = \exp\{\underset{\sim}{k}^2 G_{zz}(|\tau-\sigma|)\} \cdot \left[1 + \frac{1}{4}\lambda\left(\underset{\sim}{k}^2-k_z^2\right)\frac{w^4}{v^4}\left(|\tau-\sigma|\right)^2 + O(\lambda^2)\right]. \tag{76}$$

Use of this result for $W(\underset{\sim}{k},\tau,\sigma)$ in Eqs. (57) and (58) and performance of the indicated operations yield

$$A = \frac{\alpha u}{\sqrt{\pi} w} \int_0^\infty du \, \frac{e^{-u}}{[J(u)]^{\frac{1}{2}}} + \frac{1}{6}\lambda \, \frac{\alpha}{\sqrt{\pi}} \, \frac{w}{v} \int_0^\infty du \, \frac{u^2 e^{-u}}{[J(u)]^{3/2}} + O(\lambda^2), \tag{77}$$

and

$$B = \frac{3}{4} \, \frac{v^2-w^2}{v} - \frac{1}{2}\lambda \, w^2 \, \frac{v^2-w^2}{v^4} + O(\lambda^2), \tag{78}$$

where

$$J(u) = -2 \, \frac{v^2}{w^2} \, G_{zz} \equiv u + \frac{v^2-w^2}{vw^2} \, (1-e^{-vu}). \tag{79}$$

It should be noted that the expression for W as obtained in Eq. (76) is a function of $|\tau-\sigma|$ rather than of τ and σ separately. Consequently in obtaining the resulting expression for A and B as given by Eqs. (77) and (78), it is convenient to change the integration variables from τ and σ to τ and $|\tau-\sigma|$. Substitution of Eq. (78) into Eq. (61) and performance of the resultant integration readily yield

$$E_o^{(o)}(\alpha,\lambda) = \frac{3}{2} \, (v-w) + \frac{1}{2}\lambda \, \frac{w^2}{v^2} + O(\lambda^2). \tag{80}$$

Substitution of Eqs. (77), (78), and (80) into Eq. (51) yields

$$E_o'(\alpha,\lambda) = [\frac{3}{4}\frac{(v-w)^2}{v} - \frac{\alpha}{\sqrt{\pi}}\frac{v}{w}\int_o^\infty du\ \frac{e^{-u}}{[J(u)]^{\frac{1}{2}}}]$$

$$+ \frac{1}{2}\lambda\ [1 - \frac{(v^2-w^2)^2}{v^4} - \frac{\alpha}{3\sqrt{\pi}}\frac{w}{v}\int_o^\infty du\ \frac{u^2e^{-u}}{[J(u)]^{3/2}}]$$

$$+ O(\lambda^2). \qquad (81)$$

In view of Inequality (44), the variational parameters v and w are to be determined by minimization of $E_o'(\alpha,\lambda)$. Minimization of $E_o'(\alpha,\lambda)$ as given in expanded form by Eq. (81) yields

$$E_o'(\alpha,\lambda) = E_o'(\alpha) + \frac{1}{2}\frac{\lambda}{\mu'(\alpha)} + O(\lambda^2), \qquad (82)$$

where

$$E_o'(\alpha) \equiv E_F(\alpha) = \frac{3}{4}\frac{(v-w)^2}{v} - \frac{\alpha}{\sqrt{\pi}}\frac{v}{w}\int_o^\infty du\ \frac{e^{-u}}{[J(u)]^{\frac{1}{2}}}, \qquad (83)$$

and

$$\mu'(\alpha) = [1 - (1 - \frac{w^2}{v^2})^2 - \frac{\alpha}{3\sqrt{\pi}}\frac{w}{v}\int_o^\infty du\ \frac{u^2e^{-u}}{[J(u)]^{3/2}}]^{-1}, \qquad (84)$$

wherein the values of v and w are just those which minimize Feynman's polaron self-energy, given by Eq. (83), and have already been evaluated numerically by Schultz.[20] Comparison of Eq. (82) with Eq. (13) shows that Eqs. (83) and (84) give the polaron self-energy and effective mass in the present approximation. For comparison Feynman's polaron effective mass may be expressed as[19]

$$m_F(\alpha) = 1 + \frac{\alpha}{3\sqrt{\pi}} \frac{v^3}{w^3} \int_0^\infty du \, \frac{u^2 e^{-u}}{[J(u)]^{3/2}} . \qquad (85)$$

CHAPTER 4

RESULTS AND CONCLUSION

It is shown in Appendix E that for small α, the optimizing values of the variational parameters v and w and the polaron effective mass in the present calculation can be expanded in the form

$$v = 3 + (2/9)\alpha + O(\alpha^2), \tag{86}$$

$$w = 3 + O(\alpha), \tag{87}$$

and

$$\mu'(\alpha) = 1 + (1/6)\alpha + (73/2916)\alpha^2 + O(\alpha^3) \tag{88}$$

$$= 1 + .166667\alpha + .025034\alpha^2 + O(\alpha^3). \tag{89}$$

The weak coupling expansion of Feynman's polaron effective mass is given by[19]

$$m_F = 1 + (1/6)\alpha + (72/2916)\alpha^2 + O(\alpha^3) \tag{90}$$

$$= 1 + .166667\alpha + .024691\alpha^2 + O(\alpha^3). \tag{91}$$

For weak coupling, therefore, $m_F(\alpha)$ and $\mu'(\alpha)$ differ only slightly. It is also interesting to compare the results

of the present calculation with the fourth-order perturbation results[25]

$$\mu(\alpha) = 1 + \frac{1}{6}\alpha + \eta\alpha^2 + O(\alpha^3), \tag{92}$$

where

$$\eta = [\frac{7}{36} - \frac{5}{8}\sqrt{2} + \frac{4}{3}\ln(1+\sqrt{2}) - \frac{2}{3}\ln 2] \simeq .0236276. \tag{93}$$

An inspection of Eqs. (88)-(93) shows that the results μ' and m_F agree with the perturbation result, μ, to first order in α but that the α^2 terms in μ' and m_F are slightly higher than the corresponding α^2 term in μ, which is exact.

Similarly for large α, it is shown in Appendix E that

$$v = (4\alpha^2/9\pi) + O(\alpha^0), \tag{94}$$

$$w = 1 + O(\alpha^{-2}), \tag{95}$$

and

$$\mu'(\alpha) = m_F = (16\alpha^4/81\pi^2) + O(\alpha^{-2}). \tag{96}$$

Thus for strong coupling, $\mu'(\alpha)$ agrees with Feynman's result to the leading order in α.

For intermediate values of α, numerical evaluations are required for the two integrals occuring in Eqs. (83)-(85). A computer program was written to minimize $E_F(\alpha)$ with respect to v and w and to calculate the corresponding results for the polaron self-energy, $E_F(\alpha)$, and the effective masses $\mu'(\alpha)$ and $m_F(\alpha)$ as given by Eqs. (84) and (85). The results are shown in Table I.

Table I. Numerical results for variational parameters, self-energy and effective mass values.

α	v	w	POLARON SELF-ENERGY	POLARON EFFECTIVE MASS $\mu'(\alpha)$	$m_F(\alpha)$	$\frac{\mu'-m_F}{m_F}$ (%)
1	3.10962	2.87067	-1.01303	1.19594	1.19551	0.04
3	3.42129	2.56030	-3.13333	1.89530	1.88895	0.34
5	4.03434	2.14002	-5.44014	3.91976	3.88562	0.88
7	5.80989	1.60365	-8.11269	14.5298	14.3941	0.94
9	9.85025	1.28230	-11.4858	63.0050	62.7515	0.40
11	15.4132	1.16209	-15.7098	183.433	183.125	0.17
15	30.0822	1.07629	-26.7249	797.845	797.498	0.04

The optimum values of the parameters v and w have already been reported by Schultz,[20] but were recalculated accurately to eight significant digits in order to obtain the

percentage difference between $\mu'(\alpha)$ and m_F accurately to two places after the decimal. The results shown in Table I have been rounded off and are accurate to the number of significant figures reported. The values obtained for v and w are in slight disagreement with the values reported by Schultz,[20] but agree with the independent calculation of Marshall and Mills.[26]

In summary, Feynman's method of approximating the ground-state energy of a free polaron has been extended to approximate the ground-state energy of a polaron in a weak magnetic field. The result provides a means of approximating the polaron effective mass based on a definition which is exactly equivalent to Fröhlich's definition of the free polaron effective mass. The effective mass, $\mu'(\alpha)$, thereby obtained is slightly higher (by less than 1%) than Feynman's result, which was based on the same two-parameter model, but which was determined from Feynman's alternative, rather ad hoc definition.

The present work is similar to a calculation of the polaron effective mass by Hellwarth and Platzman.[22] Their method, which is based on the same two-parameter model employed here, involves approximating the free energy, $F(\theta,\lambda)$, of a polaron in a magnetic field as a function of temperature, θ, and of the magnetic field strength, λ. The free energy has greater informational content than the ground state energy, but is more complicated to

determine accurately. Hellwarth and Platzman's polaron effective mass, m_H, is defined by

$$m_H^{-2} = 24 \lim_{\theta \to 0} \kappa\theta \{\lim_{\lambda \to 0} F(\theta,\lambda)/\lambda^2\}, \tag{97}$$

where κ is Boltzmann's constant. This definition is also an exact prescription since for a weak magnetic field and for low temperature, the free energy is determined by the low-lying energy spectrum of a polaron in a magnetic field and since this spectrum has the same form as the energy spectrum of the motion in a magnetic field of a particle with the self-energy and effective mass of a free polaron. Their result is slightly lower than the Feynman-Schultz result (by at most 1.5%) and may be expressed as

$$m_H^{-2} = (3m_o - 2m_F)m_o^{-3} , \tag{98}$$

where m_o and m_F are Feynman's polaron mass as calculated in zeroth- and first-order in (S-S'). For the two-parameter model,

$$m_o = v^2/w^2 . \tag{99}$$

For sake of comparison, the present result may be written in the form

$$\mu'(\alpha)^{-1} = (2m_o - m_F)m_o^{-2} \quad . \tag{100}$$

Hellwarth and Platzman also discuss a generalization of the two-parameter model in which the terms of S' involving the variational parameters C and w are generalized by replacement of C by a variational function C(w') and integration over w'. For this generalization, Hellwarth and Platzman point out that Eq. (98) still holds. However, the numerical results would be much more difficult to obtain since the corresponding ground-state energy now has to be minimized with respect to the function C(w'). Hellwarth and Platzman further conclude that when the generalized model is fully optimized, $m_o \to m_F$, which upon use of Eq. (98) yields $m_F = m_o = m_H$. It may be added that Relation (100) can also be trusted for this generalized model. Therefore, upon full optimization, the generalized model yields $m_F = m_o = m_H = \mu'$. The method of Feynman's zeroth-order mass calculation can be readily extended to yield

$$m_o = 1 + 4\int_o^\infty w'^{-3}\, C(w')dw', \tag{101}$$

for the generalized model.

APPENDIX A

FRÖHLICH'S POLARON MODEL

Consider the motion of a single conduction electron of mass, m_{el}, introduced into a semiconductive ionic crystal lattice which is otherwise free from conduction electrons. If only electrostatic interactions are considered, the total energy of the electron located at the position $\underset{\sim}{r}$, is

$$E = \underset{\sim}{p}^2/(2m_{el}) + V_{Total}(\underset{\sim}{r}), \tag{A1}$$

where $\underset{\sim}{p}$ is the momentum of the electron and $V_{Total}(\underset{\sim}{r})$ is the potential energy of the electron due to all the ions of the lattice. If $V_B(\underset{\sim}{r})$ represents the value $V_{Total}(\underset{\sim}{r})$ would have if all the ions were at rest at their lattice sites, then Eq. (A1) can be written as

$$E = \underset{\sim}{p}^2/(2m_{el}) + V_B(\underset{\sim}{r}) + \Delta V(\underset{\sim}{r}), \tag{A2}$$

where

$$\Delta V = V_{Total}(\underset{\sim}{r}) - V_B(\underset{\sim}{r}). \tag{A3}$$

The Bloch approximation,[1] that all the ions are rigidly attached to their lattice sites implies that

$\Delta V(\underset{\sim}{r}) = 0$. The result of this approximation is that, measured from the bottom of the conduction band,

$$E \equiv E_{\underset{\sim}{k}} = \frac{1}{2m} p^2 = \frac{\hbar^2 k^2}{2m} . \qquad \text{(A4)}$$

where m is a constant called the band mass, not necessarily equal to the electron mass and where $\underset{\sim}{k}$ is the wave vector of the electron. Equation (A4) is valid only for the wavevector, $\underset{\sim}{k}$, small relative to the reciprocal lattice spacings.

In developing a Hamiltonian operator for this system consisting of a slowly moving conduction electron interacting with the lattice modes that the electron can significantly excite, Fröhlich[2] postulates that the result, Eq. (A4), of the Bloch's approximation can be improved upon by simply adding onto Eq. (A4) the term $\Delta V(\underset{\sim}{r})$, which has been neglected in the beginning of the Bloch treatment. Then

$$E = \frac{1}{2m} \underset{\sim}{p}^2 + \Delta V(\underset{\sim}{r}), \qquad \text{(A5)}$$

where $\Delta V(\underset{\sim}{r})$ is given by Eq. (A3). The contribution of the i^{th} lattice site to the difference, $\Delta V(\underset{\sim}{r})$ is just the difference between the potential energy of the electron due to the i^{th} ion when displaced from its lattice site and the potential energy of the electron due to the i^{th}

ion when fixed at its lattice site. For ion displacements small compared to the lattice spacings, this contribution has the form of the product of the electron charge, -e, and the electrostatic potential due to an electric dipole at the i^{th} lattice site.

The conduction electron will deform the ions in addition to displacing them from their lattice sites. However, the relaxation time for the ionic deformation is short compared to that of the displacement field so that for a slowly moving electron the deformation field relaxes much more quickly toward the spherically symmetric configuration it would have if the electron were at rest. Since a spherically symmetrical field cannot exert a force on the electron, the effect of the deformation upon the electrons motion is negligible compared to that of the displacement field.

Since for a slowly moving electron, $\underset{\sim}{k}$ is small relative to the reciprocal lattice spacings, the wave function for the Bloch electron will vary slowly over the distance of many lattice spacings. Therefore the medium can be regarded as continuous, with the result that the electric field due to the lattice can be described by a macroscopic continuous polarization field, $\underset{\sim}{P}(\underset{\sim}{r}')$.

According to the definition of the electric displacement, $\underset{\sim}{D}(\underset{\sim}{r}')$, the polarization field is related to the total electric field intensity, $\underset{\sim}{E}(\underset{\sim}{r}')$, by

$$\underset{\sim}{E}(\underset{\sim}{r}') = \underset{\sim}{D}(\underset{\sim}{r}') - 4\pi\underset{\sim}{P}(\underset{\sim}{r}'). \tag{A6}$$

Therefore, $[-4\pi\underset{\sim}{P}(\underset{\sim}{r}')]$ is the contribution made by the medium to the total electric field intensity. Since the polarization field, $\underset{\sim}{P}(\underset{\sim}{r}')$, due to ionic displacement accounts for the major force acting on the Bloch electron, the classical equation of motion of the electron of the electron is

$$m\ddot{\underset{\sim}{r}} = -e[-4\pi\underset{\sim}{P}(\underset{\sim}{r})]. \tag{A7}$$

Since the charge of the electron is the only free charge present

$$\underset{\sim}{D}(\underset{\sim}{r}') = e\nabla_{\underset{\sim}{r}'}(|\underset{\sim}{r}-\underset{\sim}{r}'|^{-1}) \tag{A8}$$

and

$$\nabla\cdot\underset{\sim}{D}(\underset{\sim}{r}') = -4\pi e\delta(\underset{\sim}{r}-\underset{\sim}{r}'). \tag{A9}$$

The potential energy, E_I, of interacting between the electron and the electric field, $[-4\pi\underset{\sim}{P}(\underset{\sim}{r}']$, due to ionic displacement polarization is given by

$$\begin{aligned} E_I &= \frac{1}{4\pi}\int d^3\underset{\sim}{r}'\ \underset{\sim}{D}(\underset{\sim}{r}').[-4\pi\underset{\sim}{P}(\underset{\sim}{r}')] \\ &= -\int d^3\underset{\sim}{r}'\ \underset{\sim}{D}(\underset{\sim}{r}')\cdot\underset{\sim}{P}(\underset{\sim}{r}'). \end{aligned} \tag{A10}$$

It is useful to observe that since the electric field, $\underset{\sim}{D}$, of the electron is longitudinal, the electron will produce only a longitudinal polarization field. Assuming that there is no transverse polarization field present to begin with, then $\underset{\sim}{P}(\underset{\sim}{r})$ will be purely longitudinal. Thus

$$\underset{\sim}{\nabla}x\underset{\sim}{P}(\underset{\sim}{r}) = \underset{\sim}{0} \tag{A11}$$

and consequently, the electric field due to polarization, $-4\pi\underset{\sim}{P}(\underset{\sim}{r})$, can be expressed in terms of its scalar potential, $\phi(\underset{\sim}{r})$ as

$$-4\pi\underset{\sim}{P}(\underset{\sim}{r}) = -\underset{\sim}{\nabla}_{\underset{\sim}{r}}\phi(\underset{\sim}{r}). \tag{A12}$$

The longitudinal modes of the lattice that produce the polarization field, are of two kinds, the acoustical-like modes and the optical-like modes. For an acoustical mode of a given wavelength, all the ions within the region between two successive nodal planes are displaced in the same direction. Therefore, since adjacent ions are oppositely charged, the resulting adjacent dipoles within such a region cancel extensively and are neglected. For an optical mode, the ions between successive nodal planes are displaced in opposite directions and therefore produce adjacent dipole moments which add constructively. The

resultant polarization is relatively large, especially for the long wavelength optical modes.

The conclusion of this discussion of modes is that only the longitudinal optical modes, and of them especially those of long wavelength, significantly interact with the electron. This is a simplifying result because these modes have a vibrational frequency, ω, which is approximately constant. Consequently, in the absence of the interaction with the electron, the polarization field, $\underset{\sim}{P}(\underset{\sim}{r}')$, resulting from the long wavelength longitudinal optical modes would obey the equation of motion

$$\ddot{\underset{\sim}{P}}(\underset{\sim}{r}') + \omega^2 \underset{\sim}{P}(\underset{\sim}{r}') = 0, \tag{A13}$$

corresponding to the Lagrangian

$$L_o(\underset{\sim}{P},\dot{\underset{\sim}{P}}) = \frac{1}{2} m_F \int d^3\underset{\sim}{r}' [\dot{\underset{\sim}{P}}^2(\underset{\sim}{r}') - \omega^2 \underset{\sim}{P}^2(\underset{\sim}{r}')] + E_z, \tag{A14}$$

where E_z is an arbitrary constant which will be chosen for convenience later and m_F is a constant which can be determined by the following considerations: In view of Eq. (A10) if a given electric displacement field, $\underset{\sim}{D}(\underset{\sim}{r}')$, is present then the Lagrangian for the polarization field would be

$$L(\underset{\sim}{P},\dot{\underset{\sim}{P}}) = L_o(\underset{\sim}{P},\dot{\underset{\sim}{P}}) + \int d^3\underset{\sim}{r}' [\underset{\sim}{P}(\underset{\sim}{r}') \cdot \underset{\sim}{D}(\underset{\sim}{r}')]. \tag{A15}$$

The equation of motion resulting from Eq. (A15) is

$$\ddot{\underset{\sim}{P}}(\underset{\sim}{r}') + \omega^2 \underset{\sim}{P}(\underset{\sim}{r}') = \frac{1}{m_F} \dot{\underset{\sim}{D}}(\underset{\sim}{r}'). \tag{A16}$$

The total polarization field, $\underset{\sim}{P}_{Total}$, can be written as

$$\underset{\sim}{P}_{Total} = \underset{\sim}{P} + \underset{\sim}{P}', \tag{A17}$$

where $\underset{\sim}{P}$ represents the field due to ionic displacement and $\underset{\sim}{P}'$ is the field due to deformation of the ions. If a static electric field is applied to the medium, then by definition of the static dielectric constant, ε,

$$4\pi \underset{\sim}{P}_{Total} = \left[1 - \frac{1}{\varepsilon}\right] \underset{\sim}{D}_s \tag{A18}$$

where $\underset{\sim}{D}_s$ is the static electric displacement field. It is known empirically that the natural frequency, ω, of the long wavelength longitudinal optical modes is in the infrared region and that the natural frequency, ω', of $\underset{\sim}{P}'$ is in the ultraviolet region. If an alternating field whose frequency lies in the visible range is applied to the medium, the polarization due to the displacement of ions will be negligible because the ions simply cannot follow the applied field. However, the ionic deformations can easily follow this field in the same way as they would for a static applied field. Therefore, in a static applied

field,

$$4\pi \underset{\sim}{P}' = [1 - \frac{1}{\varepsilon_\infty}] \underset{\sim}{D}_S \ , \tag{A19}$$

where ε_∞ is the dielectric constant measured in the visible region. Subtraction of Eq. (A18) from Eq. (A19) yields

$$4\pi \underset{\sim}{P} = [\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon}] \underset{\sim}{D}_S \ . \tag{A20}$$

Comparison of this result with Eq. (A16) for the static case, $\underset{\sim}{D} = \underset{\sim}{D}_S$ and $\dot{\underset{\sim}{P}}=0$, yields

$$\frac{1}{m_F} = \frac{\omega^2}{4\pi} (\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon}) \ . \tag{A21}$$

The total Lagrangian, L, for the electron, the long wavelength longitudinal optical modes, and the interaction between them can be obtained by combining the kinetic energy of the electron with Eq. (A15) to get

$$L(\underset{\sim}{r},\dot{\underset{\sim}{r}},\underset{\sim}{P},\dot{\underset{\sim}{P}}) = \frac{1}{2} m\dot{\underset{\sim}{r}}^2 + \frac{1}{2} m_F \int [\dot{\underset{\sim}{P}}^2(\underset{\sim}{r}') - \omega^2 \underset{\sim}{P}^2(\underset{\sim}{r}')] d^3r' + E_z$$

$$+ \int d^3\underset{\sim}{r}' [\underset{\sim}{P}(\underset{\sim}{r}') \cdot \underset{\sim}{D}(\underset{\sim}{r}')] , \tag{A22}$$

where $\underset{\sim}{P}$ is the polarization field due to the long wavelength longitudinal optical modes of frequency ω, which has been assumed to be constant, $\underset{\sim}{r}$ is the electron

coordinate, m_F is given by Eq. (A21) and $\underset{\sim}{D}$ is given by Eq. (A8).

It has been found convenient to use a natural system of units in which $m=\omega=\hbar=1$, so that the Lagrangian given by Eq. (A22) may be rewritten as

$$L(\underset{\sim}{r},\dot{\underset{\sim}{r}},\underset{\sim}{P},\dot{\underset{\sim}{P}}) = \frac{1}{2}\,\dot{\underset{\sim}{r}}^2 + \frac{1}{2}\,m_F\int d^3\underset{\sim}{r}'[\dot{\underset{\sim}{P}}^2(\underset{\sim}{r}')-\underset{\sim}{P}^2(\underset{\sim}{r}')]$$

$$+ E_z + \int d^3\underset{\sim}{r}'[\underset{\sim}{P}(\underset{\sim}{r}')\cdot\underset{\sim}{D}(\underset{\sim}{r}')]. \qquad \text{(A23)}$$

The Hamiltonian for the system is therefore given by

$$H(\underset{\sim}{r},\underset{\sim}{p},\underset{\sim}{P},\underset{\sim}{\Pi}) = \frac{\underset{\sim}{p}^2}{2} + \int d^3\underset{\sim}{r}'[\frac{1}{2}\,\frac{\underset{\sim}{\Pi}^2(\underset{\sim}{r}')}{m_F} + \frac{1}{2}\,m_F\,\underset{\sim}{P}^2(\underset{\sim}{r}')]$$

$$- E_z - \int d^3\underset{\sim}{r}'[\underset{\sim}{P}(\underset{\sim}{r}')\cdot\underset{\sim}{D}(\underset{\sim}{r}')], \qquad \text{(A24)}$$

where $\underset{\sim}{p} = m\dot{\underset{\sim}{r}}$ is the momentum conjugate to $\underset{\sim}{r}$ and $\underset{\sim}{\Pi}(\underset{\sim}{r})$ is the momentum conjugate to $\underset{\sim}{P}(\underset{\sim}{r})$ and is given by

$$\underset{\sim}{\Pi}(\underset{\sim}{r}) = m_F\dot{\underset{\sim}{P}}(\underset{\sim}{r}). \qquad \text{(A25)}$$

The canonically conjugate variables $\underset{\sim}{p}$ and $\underset{\sim}{r}$ and the canonically conjugate variables $\underset{\sim}{\Pi}$ and $\underset{\sim}{P}$ obey the Poisson's Bracket relationships

$$\{\underset{\sim}{p}_j,\ \underset{\sim}{r}_{j'}\} = \delta_{jj'} \qquad \text{(A26)}$$

and

$$\{P_j(\underset{\sim}{r}),\Pi_{j'}(\underset{\sim}{r}')\} = \delta_{jj'}\delta(\underset{\sim}{r}-\underset{\sim}{r}'). \tag{A27}$$

In order to cast the Hamiltonian in a form which is more readily convertible into a quantum-mechanical Hamiltonian operator, one may begin by introducing a complex field $\underset{\sim}{B}(\underset{\sim}{r})$, which is a linear combination of $\underset{\sim}{P}(\underset{\sim}{r})$ and $\underset{\sim}{\Pi}(\underset{\sim}{r})$, and is given by

$$\underset{\sim}{B}(\underset{\sim}{r}) = \frac{1}{i\sqrt{2m_F}}[\underset{\sim}{\Pi}(\underset{\sim}{r})-im_F\underset{\sim}{P}(\underset{\sim}{r})] \tag{A28}$$

and

$$B^*(\underset{\sim}{r}') = -\frac{1}{i\sqrt{2m_F}}[\underset{\sim}{\Pi}(\underset{\sim}{r})+im_F\underset{\sim}{P}(\underset{\sim}{r})]. \tag{A29}$$

Inverting Eqs. (A28) and (A29) one obtains

$$\underset{\sim}{P}(\underset{\sim}{r}) = -(\frac{1}{2m_F})^{\frac{1}{2}}[\underset{\sim}{B}^*(\underset{\sim}{r}) + \underset{\sim}{B}(\underset{\sim}{r})] \tag{A30}$$

and

$$\underset{\sim}{\Pi}(\underset{\sim}{r}) = -(\frac{m_F}{2})^{\frac{1}{2}}i[\underset{\sim}{B}^*(\underset{\sim}{r}) - \underset{\sim}{B}(\underset{\sim}{r})]. \tag{A31}$$

In view of Eq. (A11) it is readily verified that

$$\nabla \times \underset{\sim}{B} = \nabla \times \underset{\sim}{B}^* = \underset{\sim}{0} \tag{A32}$$

so that by subjecting $\underset{\sim}{B}$ to periodic boundary conditions on the surface of a cubical normalization volume, V, one may express $\underset{\sim}{B}$ (and $\underset{\sim}{B}^*$) in the expansion form

$$\underset{\sim}{B}(\underset{\sim}{r}) = \frac{1}{\sqrt{V}} \sum_{\underset{\sim}{k}} \frac{\underset{\sim}{k}}{|\underset{\sim}{k}|} b_{\underset{\sim}{k}} e^{i\underset{\sim}{k}\cdot\underset{\sim}{r}} \tag{A33}$$

and

$$\underset{\sim}{B}^*(\underset{\sim}{r}) = \frac{1}{\sqrt{V}} \sum_{\underset{\sim}{k}} \frac{\underset{\sim}{k}}{|\underset{\sim}{k}|} b^*_{\underset{\sim}{k}} e^{-i\underset{\sim}{k}\cdot\underset{\sim}{r}} , \tag{A34}$$

where

$$b_{\underset{\sim}{k}} = \frac{1}{\sqrt{V}} \frac{\underset{\sim}{k}}{|\underset{\sim}{k}|} \cdot \int d^3\underset{\sim}{r}\ \underset{\sim}{B}(\underset{\sim}{r}) e^{-i\underset{\sim}{k}\cdot\underset{\sim}{r}} , \tag{A35}$$

and

$$b_{\underset{\sim}{k}} = \frac{1}{\sqrt{V}} \frac{\underset{\sim}{k}}{|\underset{\sim}{k}|} \cdot \int d^3\underset{\sim}{r}\ \underset{\sim}{B}^*(\underset{\sim}{r}) e^{i\underset{\sim}{k}\cdot\underset{\sim}{r}} , \tag{A36}$$

and where the components, k_i, of the summation index $\underset{\sim}{k}$ satisfy

$$k_i = \frac{2\pi}{V^{1/3}} n_i \tag{A37}$$

with

$$n_i = 0, \pm 1, \pm 2, \text{----}. \tag{A38}$$

The limit $V \to \infty$ is to be taken, whereupon

$$\sum_{\underset{\sim}{k}} \to \frac{V}{(2\pi)^3} \int d^3\underset{\sim}{k} . \tag{A39}$$

In view of the fact that $\underset{\sim}{P}$ and $\underset{\sim}{\Pi}$ are real, Eqs. (A28), (A29), (A35), and (A36) imply that

$$b^*_{\underset{\sim}{k}} = -b_{-\underset{\sim}{k}} . \tag{A40}$$

Substitution of Eqs. (A33) and (A34) into Eqs. (A30) and (A31) yields

$$\underset{\sim}{P}(\underset{\sim}{r}) = -\left(\frac{1}{2m_F V}\right)^{\frac{1}{2}} \sum_{\underset{\sim}{k}} \frac{\underset{\sim}{k}}{|\underset{\sim}{k}|} \left[b^*_{\underset{\sim}{k}} e^{-i\underset{\sim}{k}\cdot\underset{\sim}{r}} + b_{\underset{\sim}{k}} e^{i\underset{\sim}{k}\cdot\underset{\sim}{r}}\right] \tag{A41}$$

and

$$\underset{\sim}{\Pi}(\underset{\sim}{r}) = -\left(\frac{m_F}{2V}\right)^{\frac{1}{2}} \sum_{\underset{\sim}{k}} \frac{\underset{\sim}{k}}{|\underset{\sim}{k}|} i\left[b^*_{\underset{\sim}{k}} e^{-i\underset{\sim}{k}\cdot\underset{\sim}{r}} - b_{\underset{\sim}{k}} e^{-i\underset{\sim}{k}\cdot\underset{\sim}{r}}\right]. \tag{A42}$$

By use of Eqs. (A27), (A30), and (A31) it is straightforward to show that

$$\{\mathcal{B}_j(\underset{\sim}{r}), \mathcal{B}^*_{j'}(\underset{\sim}{r}')\} = -i\delta_{jj'}\delta(\underset{\sim}{r}-\underset{\sim}{r}'). \tag{A43}$$

From Eqs. (A33), (A34), and (A43) one obtains

$$\{b_{\underset{\sim}{k}}, b^{*}_{\underset{\sim}{k}'}\} = -i\delta_{\underset{\sim}{k},\underset{\sim}{k}'} \tag{A44}$$

and

$$\{b_{\underset{\sim}{k}}, b_{\underset{\sim}{k}'}\} = \{b^{+}_{\underset{\sim}{k}}, b^{+}_{\underset{\sim}{k}'}\} = 0. \tag{A45}$$

By use of Eqs. (A9) and (A12), the last term of the Hamiltonian, given by Eq. (A24), can be rewritten as

$$\begin{aligned} -\int d^3\underset{\sim}{r}'\ \underset{\sim}{D}(\underset{\sim}{r}')\cdot\underset{\sim}{P}(\underset{\sim}{r}') &= -\frac{1}{4\pi}\int d^3\underset{\sim}{r}'\ \underset{\sim}{D}(\underset{\sim}{r}')\cdot\nabla_{\underset{\sim}{r}}\phi(\underset{\sim}{r}') \\ &= \frac{1}{4\pi}\int d^3\underset{\sim}{r}'\ \phi(\underset{\sim}{r}')\nabla_{\underset{\sim}{r}'}\cdot\underset{\sim}{D}(\underset{\sim}{r}') \\ &= -e\phi(\underset{\sim}{r}) \ . \end{aligned} \tag{A46}$$

It is readily verified that

$$\phi(\underset{\sim}{r}) = -4\pi i\left(\frac{1}{2m_F V}\right)^{\frac{1}{2}} \sum_{\underset{\sim}{k}} \frac{1}{|\underset{\sim}{k}|}\left[b^{*}_{\underset{\sim}{k}}\, e^{-i\underset{\sim}{k}\cdot\underset{\sim}{r}} - b_{\underset{\sim}{k}} e^{i\underset{\sim}{k}\cdot\underset{\sim}{r}}\right] \tag{A47}$$

satisfies Eq. (A12), where $\underset{\sim}{P}$ is given by Eq. (A41). Substitution of Eqs. (A28), (A29), and (A46) into Eq. (A24) yields

$$H = \frac{1}{2}\,\underset{\sim}{p}^2 + \int d^3r'\ \underset{\sim}{B}^{*}(\underset{\sim}{r}')\cdot\underset{\sim}{B}(\underset{\sim}{r}') - E_z - e\phi(\underset{\sim}{r}). \tag{A48}$$

By using Eqs. (A33), (A34), and (A47), one may rewrite

Eq. (A48) as follows:

$$H = \frac{1}{2}\,\underset{\sim}{p}^2 + \frac{1}{2}\sum_{\underset{\sim}{k}} [b^*_{\underset{\sim}{k}} b_{\underset{\sim}{k}} + b_{\underset{\sim}{k}} b^*_{\underset{\sim}{k}}] - E_z$$

$$+ 4\pi i e \left(\frac{1}{2m_F V}\right)^{1/2} \sum_{\underset{\sim}{k}} \frac{1}{|\underset{\sim}{k}|} [b^*_{\underset{\sim}{k}}\, e^{-i\underset{\sim}{k}\cdot\underset{\sim}{r}} - b_{\underset{\sim}{k}}\, e^{i\underset{\sim}{k}\cdot\underset{\sim}{r}}]. \quad \text{(A49)}$$

This equation has been written in symmetrized form appropriate for obtaining the quantum-mechanical Hamiltonian operator. This quantization is achieved by replacing $\underset{\sim}{p}$ by $i\nabla_{\underset{\sim}{r}}$, by replacing $b_{\underset{\sim}{k}}$ and $b^*_{\underset{\sim}{k}}$ by operators $b_{\underset{\sim}{k}}$ and $b^+_{\underset{\sim}{k}}$, and by replacing Poisson Brackets by -i times the corresponding commutator. Equations (A44) and (A45) then become

$$[b_{\underset{\sim}{k}}, b^+_{\underset{\sim}{k}'}] = \delta_{\underset{\sim}{k}\underset{\sim}{k}'}, \quad \text{(A50)}$$

and

$$[b_{\underset{\sim}{k}}, b_{\underset{\sim}{k}'}] = [b^+_{\underset{\sim}{k}}, b^+_{\underset{\sim}{k}'}] = 0, \quad \text{(A51)}$$

whereas Eq. (A49) becomes

$$H = -\frac{1}{2}\,\nabla^2_{\underset{\sim}{r}} + \sum_{\underset{\sim}{k}} b^+_{\underset{\sim}{k}} b_{\underset{\sim}{k}}$$

$$+ i\left(\frac{2\sqrt{2\pi\alpha}}{V}\right)^{1/2} \sum_{\underset{\sim}{k}} \frac{1}{|\underset{\sim}{k}|} [b^*_{\underset{\sim}{k}}\, e^{-i\underset{\sim}{k}\cdot\underset{\sim}{r}} - b_{\underset{\sim}{k}}\, e^{i\underset{\sim}{k}\cdot\underset{\sim}{r}}], \quad \text{(A52)}$$

wherein α is the polaron coupling constant given by*

$$\alpha = \frac{e^2}{2}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon}\right) = \frac{4\pi}{\sqrt{2}}\frac{e^2}{m_F} \tag{A53}$$

and where use has been made of Eqs. (A50) and (A51) and where the arbitrary constant E_z has been set equal to the zero-point energy

$$E_z = \frac{1}{2}\sum_{\underset{\sim}{k}} 1 \tag{A54}$$

of the polarization field in the absence of interaction with the electron. The first term in Eq. (A52) is the kinetic energy of the electron (of band mass 1), the second term is the energy of all the longitudinal phonons ($b^+_{\underset{\sim}{k}} b_{\underset{\sim}{k}}$ being the number operator for a phonon of wavevector $\underset{\sim}{k}$), and the third term is the electron -LO- phonon interaction. In view of the form of Eq. (A52) and the Bosonic commutation rules expressed by Eqs. (A50) and (A51), $b^+_{\underset{\sim}{k}}$ and $b_{\underset{\sim}{k}}$ are phonon creation and destruction operators.

It is also sometimes useful to regard the polaron Hamiltonian as representing a system of oscillators rather than a system consisting of phonons. To do so one may express the polarization field given by Eq. (A41) as

---

* The polaron coupling constant, α, is expressed in ordinary units by Eq. (2).

$$\underset{\sim}{P}(\underset{\sim}{r}) = -\left(\frac{1}{2m_F V}\right)^{\frac{1}{2}} \{\sum_{k\epsilon S_1} \frac{\underset{\sim}{k}}{|\underset{\sim}{k}|} [(b_{\underset{\sim}{k}}+b^*_{\underset{\sim}{k}})\cos(\underset{\sim}{k}\cdot\underset{\sim}{r})$$

$$+ i(b_{\underset{\sim}{k}}-b^*_{\underset{\sim}{k}})\sin(\underset{\sim}{k}\cdot\underset{\sim}{r})] + \sum_{k\epsilon S_u} \frac{\underset{\sim}{k}}{|\underset{\sim}{k}|}[(b_{\underset{\sim}{k}}+b^*_{\underset{\sim}{k}})\cos(\underset{\sim}{k}\cdot\underset{\sim}{r})$$

$$+ i(b_{\underset{\sim}{k}}-b^*_{\underset{\sim}{k}})\sin(\underset{\sim}{k}\cdot\underset{\sim}{r})]\}, \qquad \text{(A55)}$$

where $\underset{\sim}{k}\epsilon S_u$ means that $\underset{\sim}{k}$ has at least one positive rectangular component and $\underset{\sim}{k}\epsilon S_1$ means $k\notin S_u$. By introducing the notation $\{{X(\underset{\sim}{k}) \atop Y(\underset{\sim}{k})}\}$ to stand for $X(\underset{\sim}{k})$ if $\underset{\sim}{k}\epsilon S_u$ and $Y(\underset{\sim}{k})$ if $\underset{\sim}{k}\epsilon S_1$ and by using Eq. (40), one may write Eq. (A55) as

$$\underset{\sim}{P}(\underset{\sim}{r}) = \left(\frac{2}{m_F V}\right)^{\frac{1}{2}} \sum_{\underset{\sim}{k}} \frac{\underset{\sim}{k}}{|\underset{\sim}{k}|} q_{\underset{\sim}{k}} \{{+\sin \underset{\sim}{k}\cdot\underset{\sim}{r} \atop -\cos \underset{\sim}{k}\cdot\underset{\sim}{r}}\}, \qquad \text{(A56)}$$

where

$$q_{\underset{\sim}{k}} = \{{(b_{\underset{\sim}{k}}+b^*_{\underset{\sim}{k}}) \atop \frac{1}{i}(b_{\underset{\sim}{k}}-b_{\underset{\sim}{k}})}\}. \qquad \text{(A57)}$$

By use of Eq. (A12) one may readily verify that

$$\phi(\underset{\sim}{r}) = -4\pi \left(\frac{2}{m_F V}\right)^{\frac{1}{2}} \sum_{\underset{\sim}{k}} \frac{1}{|\underset{\sim}{k}|} q_{\underset{\sim}{k}} \{{\cos \underset{\sim}{k}\cdot\underset{\sim}{r} \atop \sin \underset{\sim}{k}\cdot\underset{\sim}{r}}\}. \qquad \text{(A58)}$$

Substitution of Eq. (A58) into Eq. (A46) and substitution of the result along with Eq. (A56) into Eq. (A22) lead to the result that

$$L(\underset{\sim}{r},\dot{\underset{\sim}{r}},q_{\underset{\sim}{k}},\dot{q}_{\underset{\sim}{k}}) = \frac{1}{2}\,\dot{\underset{\sim}{r}}^2 + \frac{1}{2}\sum_{\underset{\sim}{k}} (\dot{q}_{\underset{\sim}{k}}^2 - q_{\underset{\sim}{k}}^2 + 1)$$

$$- \left[\frac{8\sqrt{2}\pi\alpha}{V}\right]^{\frac{1}{2}} \sum_{\underset{\sim}{k}} \frac{1}{|\underset{\sim}{k}|}\, q_{\underset{\sim}{k}} \begin{Bmatrix} \cos \underset{\sim}{k}\cdot\underset{\sim}{r} \\ \sin \underset{\sim}{k}\cdot\underset{\sim}{r} \end{Bmatrix}. \qquad \text{(A59)}$$

This particular form for the polaron Lagrangian is convenient in the respect that the electron -LO- phonon interaction term involves the generalized coordinates, the $q_{\underset{\sim}{k}}$'s, but not also their time derivatives.

The corresponding Hamiltonian, in terms of the coordinates $\underset{\sim}{r},\{q_{\underset{\sim}{k}}\}$ and their conjugate momenta $\underset{\sim}{p},\{p_{\underset{\sim}{k}}\}$, may be obtained by the definition

$$H = \underset{\sim}{p}\cdot\dot{\underset{\sim}{r}} + \sum_{\underset{\sim}{k}} p_{\underset{\sim}{k}}\dot{q}_{\underset{\sim}{k}} - L(\underset{\sim}{r},\dot{\underset{\sim}{r}},q_{\underset{\sim}{k}},\dot{q}_{\underset{\sim}{k}}), \qquad \text{(A60)}$$

where

$$\underset{\sim}{p} = \frac{\partial L}{\partial \dot{\underset{\sim}{r}}} = \dot{\underset{\sim}{r}} \qquad \text{(A61)}$$

and

$$p_{\underset{\sim}{k}} = \frac{\partial L}{\partial \dot{q}_{\underset{\sim}{k}}} = \dot{q}_{\underset{\sim}{k}}\,. \qquad \text{(A62)}$$

The result is

$$H = \frac{1}{2}\,\underset{\sim}{p}^2 + \frac{1}{2}\sum_{\underset{\sim}{k}} (p_{\underset{\sim}{k}}^2 + q_{\underset{\sim}{k}}^2 - 1)$$

$$+ \left[\frac{8\sqrt{2}\pi\alpha}{V}\right]^{\frac{1}{2}} \sum_{\underset{\sim}{k}} \frac{1}{|\underset{\sim}{k}|}\, q_{\underset{\sim}{k}} \begin{Bmatrix} \cos \underset{\sim}{k}\cdot\underset{\sim}{r} \\ \sin \underset{\sim}{k}\cdot\underset{\sim}{r} \end{Bmatrix}. \qquad \text{(A63)}$$

If in addition a magnetic field, $\underset{\sim}{B}$, is also impressed along the z axis of the system, Eqs. (A52), (A59), and (A63) become

$$H(\alpha,\lambda) = \frac{1}{2}\left(-i\frac{\partial}{\partial \underset{\sim}{r}} + \frac{e}{c}\underset{\sim}{A}\right)^2 + \sum_{\underset{\sim}{k}} b^{+}_{\underset{\sim}{k}} b_{\underset{\sim}{k}}$$

$$+ i\left[\frac{2\sqrt{2}\pi\alpha}{V}\right]^{\frac{1}{2}} \sum_{\underset{\sim}{k}} \frac{1}{|\underset{\sim}{k}|}\left[b_{\underset{\sim}{k}} e^{-i\underset{\sim}{k}\cdot\underset{\sim}{r}} - b_{\underset{\sim}{k}} e^{i\underset{\sim}{k}\cdot\underset{\sim}{r}}\right], \quad \text{(A64)}$$

$$L(\alpha,\lambda) = \frac{1}{2}\dot{\underset{\sim}{r}}^2 - \frac{e}{c}\underset{\sim}{A}\cdot\dot{\underset{\sim}{r}} + \frac{1}{2}\sum_{\underset{\sim}{k}}\left(\dot{q}^2_{\underset{\sim}{k}} - q^2_{\underset{\sim}{k}} + 1\right)$$

$$- \left[\frac{8\sqrt{2}\pi\alpha}{V}\right]^{\frac{1}{2}} \sum_{\underset{\sim}{k}} \frac{1}{|\underset{\sim}{k}|} q_{\underset{\sim}{k}} \begin{Bmatrix} \cos \underset{\sim}{k}\cdot\underset{\sim}{r} \\ \sin \underset{\sim}{k}\cdot\underset{\sim}{r} \end{Bmatrix}, \quad \text{(A65)}$$

$$H(\alpha,\lambda) = \frac{1}{2}\left(\underset{\sim}{p} + \frac{e}{c}\underset{\sim}{A}\right)^2 + \sum_{\underset{\sim}{k}}\left(p^2_{\underset{\sim}{k}} + q^2_{\underset{\sim}{k}} - 1\right)$$

and

$$+ \left[\frac{8\sqrt{2}\pi\alpha}{V}\right]^{\frac{1}{2}} \sum_{\underset{\sim}{k}} \frac{1}{|\underset{\sim}{k}|} q_{\underset{\sim}{k}} \begin{Bmatrix} \cos \underset{\sim}{k}\cdot\underset{\sim}{r} \\ \sin \underset{\sim}{k}\cdot\underset{\sim}{r} \end{Bmatrix}, \quad \text{(A66)}$$

where

$$\underset{\sim}{B} = \nabla \underset{\sim}{x} \underset{\sim}{A}\ , \quad \text{(A67)}$$

$$\underset{\sim}{A} = \frac{c}{e}(-\lambda y, 0, 0), \quad \text{(A68)}$$

and

$$\lambda = \frac{eB}{c}\ , \quad \text{(A69)}$$

wherein c is the velocity of light.

APPENDIX B

MARSHALL-ROBERT THEOREM

It is shown in Appendix A that the motion of a polaron in a uniform magnetic field, $\underset{\sim}{B}$, impressed along the z axis of the system, can be described by means of the Hamiltonian

$$H(\alpha,\lambda) = \frac{1}{2}\left(-i\frac{\partial}{\partial \underset{\sim}{r}} + \frac{e}{c}\underset{\sim}{A}\right)^2 + \sum_{\underset{\sim}{k}} b^{+}_{\underset{\sim}{k}} b_{\underset{\sim}{k}}$$

$$+ i\left(\frac{2\sqrt{2}\pi\alpha}{V}\right)^{\frac{1}{2}} \sum_{\underset{\sim}{k}} \frac{1}{|\underset{\sim}{k}|}\left[\left(b^{+}_{\underset{\sim}{k}} e^{-i\underset{\sim}{k}\cdot\underset{\sim}{r}} - b_{\underset{\sim}{k}} e^{i\underset{\sim}{k}\cdot\underset{\sim}{r}}\right)\right], \tag{B1}$$

where -e is the electronic charge, $\underset{\sim}{r} = (x,y,z)$ is the electron position vector, $b^{+}_{\underset{\sim}{k}}$ and $b_{\underset{\sim}{k}}$ are Bosonic creation and destruction operators for a LO phonon of wave vector $\underset{\sim}{k}$, and where $\underset{\sim}{A}$ is the magnetic vector potential given by

$$\underset{\sim}{A} = \frac{c}{e}(-\lambda y, 0, 0) \tag{B2}$$

with

$$\lambda = eB/c \ . \tag{B3}$$

It is to be shown here that, for a sufficiently weak magnetic field, the lowest-lying eigenvalues of $H(\alpha,\lambda)$

are given by

$$E_n(\alpha,\lambda) = E_o(\alpha) + [\tfrac{1}{2}k_{T,z}^2 + \lambda(n+\tfrac{1}{2})]/\mu(\alpha)$$

$$+ O^2(k_{T,z}^2,\lambda), \tag{B4}$$

where $n = 0,1,2,3$----and $E_o(\alpha)$ and $\mu(\alpha)$ are exactly the self-energy and the effective mass of a free polaron as defined by Fröhlich. In Theorem (B4), $k_{T,z}$ is the z component of the polaron's total canonical wave vector given by

$$\underset{\sim}{K}_T = -i\frac{\partial}{\partial \underset{\sim}{r}} + \frac{e}{c}\underset{\sim}{A} + \sum_{\underset{\sim}{k}} \underset{\sim}{k} b_{\underset{\sim}{k}}^{+} b_{\underset{\sim}{k}}\ , \tag{B5}$$

and $O^2(k_{T,z}^2,\lambda)$ stands for terms of second and higher order jointly in $k_{T,z}^2$ and λ (including for example terms proportional to $k_{T,z}^4, \lambda^2$, and $\lambda k_{T,z}^2$).

Let U be the unitary operator defined by

$$U \equiv e^{-i\underset{\sim}{r}\cdot\underset{\sim}{w}}, \tag{B6}$$

where

$$\underset{\sim}{w} = \sum_{\underset{\sim}{k}} \underset{\sim}{k} b_{\underset{\sim}{k}}^{+} b_{\underset{\sim}{k}}\ . \tag{B7}$$

Then

$$H' \equiv U^{+}HU = H_{o} + \frac{1}{2}\underset{\sim}{K}_{T}'^{2} - \underset{\sim}{K}_{T}' \cdot \underset{\sim}{W} \ , \tag{B8}$$

where

$$\underset{\sim}{K}_{T}' \equiv U^{+}\underset{\sim}{K}_{T}U = -i\underset{\sim}{\nabla}_{\underset{\sim}{r}} - (\lambda y, 0, 0) \tag{B9}$$

and where

$$H_{o} = \frac{W^{2}}{2} + \sum_{\underset{\sim}{k}} b_{\underset{\sim}{k}}^{+} b_{\underset{\sim}{k}} + i\left(\frac{2\sqrt{2}\pi\alpha}{V}\right)^{\frac{1}{2}} \sum_{\underset{\sim}{k}} \frac{1}{|\underset{\sim}{k}|}[(b_{\underset{\sim}{k}}^{+} - b_{\underset{\sim}{k}})] \tag{B10}$$

is the Hamiltonian for a free polaron of zero total wave vector, the least eigenvalue, E_{o}, of which is the self-energy of a free polaron and is assumed to be non-degenerate and to be less than the excited energy eigenvalues of H_{o} by at least some finite energy gap, Δ. Since U is unitary, the eigenspectra of primed and the corresponding unprimed operators are equivalent. The method of derivation to be used is to treat the last term of Eq. (B8) as a perturbation to obtain the eigenvalues of H' both in the case of no magnetic field (λ=0) and in the case of a weak, non-zero, magnetic field. The former case leads to an exact expression for the free polaron effective mass. This same expression also arises in the latter case in such a way that the desired result, Eq. (B8), is obtained.

Let j = 0,1,2,... be an index to identify the members

of a complete orthonormal set of exact (but unknown) eigenfunctions of H_o so that

$$H_o|j\rangle = E_j(\alpha)|j\rangle \tag{B11}$$

with

$$E_o(\alpha) + \Delta \leq E_1(\alpha) \leq E_2(\alpha) \leq \ldots \quad . \tag{B12}$$

Then in the case $\lambda = 0$, the functions

$$|j,\underset{\sim}{k}_T\rangle = V^{-\frac{1}{2}} \exp(i\underset{\sim}{k}_T \cdot \underset{\sim}{r})|j\rangle \tag{B13}$$

satisfy the eigenequations

$$[H_o + \tfrac{1}{2}\underset{\sim}{K}_T'^2]|j,\underset{\sim}{k}_T\rangle = [E_j(\alpha) + \tfrac{1}{2}\underset{\sim}{k}_T^2]|j,\underset{\sim}{k}_T\rangle \tag{B14}$$

and

$$\underset{\sim}{K}_T'|j,\underset{\sim}{k}_T\rangle = \underset{\sim}{k}_T|j,\underset{\sim}{k}_T\rangle \ , \tag{B15}$$

and therefore represent states of a polaron with total wave vector $\underset{\sim}{k}_T = (k_{T,x}, k_{T,y}, k_{T,z})$. From perturbation theory and Eqs. (B7)-(B15), the energy of a free (ground state) polaron of total wave vector $\underset{\sim}{k}_T$ is given by

$$E_o(\alpha,\underset{\sim}{k}_T) = E_o(\alpha) + \frac{1}{2}\underset{\sim}{k}_T^2 - \underset{\sim}{k}_T \cdot \langle 0|\underset{\sim}{w}|0\rangle$$

$$- \Sigma_i k_{T,i}^2 \Sigma_j' \frac{|\langle j|w_i|0\rangle|^2}{E_j(\alpha) - E_o(\alpha)} + O^3(\underset{\sim}{k}_T), \tag{B16}$$

where the index i takes on the values x, y, and z and where the prime on the summation indicates omission of the $j = 0$ term. As a consequence of the invariance of H_o under rotation of coordinate axes, the summation over j in Eq. (B16) is independent of the coordinate axis index, i, and

$$E_o(\alpha,k_T) = E_o(\alpha) + \underset{\sim}{k}_T^2/(2\mu(\alpha)) + O(\underset{\sim}{k}_T^4), \tag{B17}$$

where

$$\mu(\alpha) = [1 - 2\Sigma_j' \frac{|\langle j|w_z|0\rangle|^2}{E_j(\alpha) - E_o(\alpha)}]^{-1} \tag{B18}$$

is, therefore, the effective mass of a free polaron in accordance with Fröhlich's definition.

In the case $\lambda \neq 0$, a complete orthonormal set, $|j,n,k_{T,x},k_{T,z}\rangle$ satisfying the eigenequations

$$[H_o + \tfrac{1}{2}K_T'^2]|j,n,k_{T,x},k_{T,y}> = [E_j(\alpha) + \tfrac{1}{2}k_{T,z}^2 + \lambda\,(n+\tfrac{1}{2})]|j,nk_{T,x},k_{T,z}>, \tag{B19}$$

$$K'_{T,x}|j,n,k_{T,x},K_{T,z}> = k_{T,x}|j,n,k_{T,x},k_{T,z}> , \tag{B20}$$

and

$$k'_{T,z}|j,n,k_{T,x},k_{T,z}> = k_{T,z}|j,n,k_{T,x},k_{T,z}> \tag{B21}$$

may be expressed by

$$|j,n,k_{T,x},k_{T,z}> = V^{-1/3} \exp i(k_{T,x}x + k_{T,z}z)\ \phi_n|j> , \tag{B22}$$

where $n = 0,1,2,\ldots$ and

$$\phi_n = (n!)^{-\frac{1}{2}}(a^+)^n\phi_o , \tag{B23}$$

wherein

$$a = \frac{1}{\sqrt{2\lambda}}\left[(y\lambda - k_{T,x}) + \frac{\partial}{\partial y}\right] \tag{B24}$$

and ϕ_o is that normalized function of y which satisfies the equation

$$a\phi_o = 0. \tag{B25}$$

Moreover,

$$-\underset{\sim}{K}'_T \cdot \underset{\sim}{w}|j,n,k_{T,x},k_{T,z}\rangle = [(\tfrac{\lambda}{2})^{\frac{1}{2}}(w_x+iw_y)a+(\tfrac{\lambda}{2})^{\frac{1}{2}}(w_x-iw_y)a^+ - k_{T,z}w_z]|j,n,k_{T,x},k_{T,z}\rangle, \tag{B26}$$

$$a^+\phi_n = (n+1)^{\frac{1}{2}}\phi_{n+1}\ , \tag{B27}$$

and

$$a\phi_n = n^{\frac{1}{2}}\ \phi_{n-1}\ . \tag{B28}$$

For a sufficiently weak magnetic field (so that λ is sufficiently small) since the energy gap Δ is a positive number independent of λ, then according to Eqs. (B8), (B12), (B19), and (B27), the lowest-lying eigenvalues of H' may be obtained as the following perturbation upon those eigenvalues of Eq. (B19) for which j = 0:

$$E_n(\alpha,\lambda) = E_o(\alpha) + \lambda(n+\tfrac{1}{2}) + \frac{1}{2}\frac{k_{T,z}^2}{\mu(\alpha)} - k_{T,z}\langle 0|w_z|0\rangle$$

$$- \frac{\lambda}{2}(n+1)\ \Sigma'_j\ \frac{|\langle j|w_x - iw_y|0\rangle|^2}{E_j(\alpha)-E_o(\alpha)+\lambda}$$

$$- \frac{\lambda}{2}\, n\Sigma'_j\ \frac{|\langle j|w_x + iw_y|0\rangle|^2}{E_j(\alpha)-E_o(\alpha)-\lambda} + O^3(k_{T,z},\sqrt{\lambda}), \qquad \text{(B29)}$$

where Eqs. (B8), (B18), (B19), (B26), (B27), and (B28) have been employed and primes have been placed on the summations over j in recognition of the fact that the summands vanish for j = 0, due to the rotational invariance of H_o. Since the denominators of Eq. (B29) do not vanish in the limit $\lambda \to 0$, the terms $\pm\lambda$ in these denominators may be dropped because the discrepancy in doing so is of order λ^2 and may be included in the last term of Eq. (B29). The Hermitian property of $\underset{\sim}{w}$ then may be used to obtain

$$E_n(\alpha,\lambda) = E_o(\alpha) + \lambda(n+\tfrac{1}{2}) + \frac{1}{2}\frac{k_{T,z}^2}{\mu(\alpha)} - k_{T,z}\langle 0|w_z|0\rangle$$

$$- \lambda\,(n+\tfrac{1}{2})\ \Sigma'_j\ \frac{|\langle j|w_x|0\rangle|^2 + |\langle j|w_y|0\rangle|^2}{E_j(\alpha) - E_o(\alpha)}$$

$$+ O^3(k_{T,z},\sqrt{\lambda}). \qquad \text{(B30)}$$

Equation (B4) is finally obtained by once more invoking the rotational invariance of H_o and by use of Eq. (B18). Equation (13) employed in the text is the special case of Eq. (B4) obtained by setting $n = k_{T,z} = 0$.

APPENDIX C

It is to be proved that for a sufficiently weak magnetic field, Inequality (44) holds, wherein $E_o(\alpha,\lambda)$ and $E_o'(\alpha,\lambda)$ are given by Eqs. (41) and (45).

The path-average of any function of path $X[\underset{\sim}{r}(t)]$, defined by Eq. (47), can be expressed in the alternative form

$$\langle X[\underset{\sim}{r}(t)]\rangle = \int_{\underset{\sim}{o},o}^{\underset{\sim}{o},T} X[\underset{\sim}{r}(t)]p[\lambda,\underset{\sim}{r}(t)]\, D\underset{\sim}{r}(t), \tag{C1}$$

where

$$p[\lambda,\underset{\sim}{r}(t)] = \frac{e^{S'}}{\int_{\underset{\sim}{o},o}^{\underset{\sim}{o},T} e^{S'} D\underset{\sim}{r}(t)}, \tag{C2}$$

where S' is given by Eq. (48). The main basis of Inequality (44) lies in the fact that for a real variable X, the curve $f_1(X) = e^X$ is always concaved away from the X axis. The tangent to the curve $f_1(X)$ at the point $X = \mathrm{Re}\langle X\rangle$ on the X axis, has the equation

$$f_2(X) = e^{\mathrm{Re}\langle X\rangle}[X - \mathrm{Re}\langle X\rangle + 1], \tag{C3}$$

so that

$$e^{X} \geq e^{\mathrm{Re}\langle X\rangle}[X - \mathrm{Re}\langle X\rangle + 1] \ . \tag{C4}$$

Let

$$X = S - S' \ , \tag{C5}$$

(which is real function of path) and let $I(\lambda)$ be the real function of λ defined by

$$I(\lambda) = \int_{\underset{\sim}{o},\underset{\sim}{o}}^{\underset{\sim}{o},T} \{e^{X} - e^{\mathrm{Re}\langle X\rangle}[X - \mathrm{Re}\langle X\rangle + 1]\} \mathrm{Re}\ p[\lambda, \underset{\sim}{r}(t)]\, D\underset{\sim}{r}(t) \ . \tag{C6}$$

Then by multiplying Inequality (C4) by $\mathrm{Re}\ p[\lambda, \underset{\sim}{r}(t)]$, path-integrating and setting $\lambda = 0$, one obtains

$$I(0) \geq 0 \ , \tag{C7}$$

because $\mathrm{Re}\ p[0, \underset{\sim}{r}(t)] = p[0, \underset{\sim}{r}(t)] \geq 0$. If it is assumed that $I(\lambda)$ is a continuous function of λ at $\lambda = 0$, then $I(\lambda) \geq 0$ for sufficiently small λ. Thus, for a sufficiently weak magnetic field,

$$\int_{\underset{\sim}{o},o}^{\underset{\sim}{o},T} e^{X} \mathrm{Re}\ p[\lambda, \underset{\sim}{r}(t)]\, D\underset{\sim}{r}(t) \geq e^{\mathrm{Re}\langle X\rangle} \int_{\underset{\sim}{o},o}^{\underset{\sim}{o},T} [X - \mathrm{Re}\langle X\rangle + 1] \cdot \mathrm{Re}\ p[\lambda, \underset{\sim}{r}(t)]\, D\underset{\sim}{r}(t) \ . \tag{C8}$$

By use of Eqs. (C1) and (C2), this result can be written in the more compact form

$$\mathrm{Re}\langle e^{X}\rangle \geq e^{\mathrm{Re}\langle X\rangle} , \tag{C9}$$

which, by use of Eqs. (47) and (C5) becomes

$$\mathrm{Re}\left(\frac{\int_{\underset{\sim}{o},\underset{\sim}{o}}^{\underset{\sim}{o},T} e^{S}\, Dr(t)}{\int_{\underset{\sim}{o},o}^{\underset{\sim}{o},T} e^{S'}\, D\underset{\sim}{r}(t)}\right) \geq e^{\mathrm{Re}\langle S-S'\rangle} . \tag{C10}$$

By taking logarithms of both sides, by using Eqs. (41) and (46) and the fact that both $E_o(\alpha,\lambda)$ and $E_o^{(o)}(\alpha,\lambda)$ are real, and by rearranging terms one obtains

$$E_o(\alpha,\lambda) \leq E_o^{(o)}(\alpha,\lambda) - \lim_{T\to\infty} T^{-1}\, \mathrm{Re}\langle S-S'\rangle . \tag{C11}$$

For a sufficiently weak magnetic field, $\langle S-S'\rangle$ was calculated in the text and was found to be real. Hence, by Eq. (45), $E_o(\alpha,\lambda) \leq E_o'(\alpha,\lambda)$ for sufficiently small λ, as was to be demonstrated.

APPENDIX D

SOLUTION OF INTEGRO-DIFFERENTIAL EQUATIONS

It is required to find the trajectory, $\underset{\sim}{r}(t)$, which satisfies the boundary conditions $\underset{\sim}{r}(o) = \underset{\sim}{r}(T) = \underset{\sim}{0}$ and the integro-differential equations

$$\ddot{\bar{x}}(t) = 2C\int_o^T e^{-w|t-s|}[\bar{x}(t)-\bar{x}(s)]ds + i\lambda\dot{\bar{y}} - f_x(\underset{\sim}{k},t,\tau,\sigma), \tag{D1}$$

$$\ddot{\bar{y}}(t) = 2C\int_o^T e^{-w|t-s|}[\bar{y}(t) - \bar{y}(s)]ds - i\lambda\dot{\bar{x}} - f_y(\underset{\sim}{k},t,\tau,\sigma), \tag{D2}$$

and

$$\dddot{\bar{z}}(t) = 2C\int_o^T e^{-w|t-s|}[\bar{z}(t) - \bar{z}(s)]ds - f_z(\underset{\sim}{k},t,\tau,\sigma) \tag{D3}$$

for $0 \leq t \leq T$, where

$$\underset{\sim}{f}(\underset{\sim}{k},t,\tau,\sigma) = i\underset{\sim}{k}[\delta(t-\tau) - \delta(t-\sigma)], \tag{D4}$$

and where C, w, and λ are constants. Since $\underset{\sim}{\bar{r}}(t)$ is used only for the determination of

$$W(\underset{\sim}{k},\tau,\sigma) = \exp\left\{\frac{1}{2}\int_0^T dt\ \underset{\sim}{f}(\underset{\sim}{k},t,\tau,\sigma)\cdot\bar{\underset{\sim}{r}}(t)\right\} \tag{D5}$$

and since

$$\int_0^T \underset{\sim}{f}(\underset{\sim}{k},t,\tau,\sigma)dt = 0, \tag{D6}$$

it is sufficient to find $\bar{\underset{\sim}{r}}(t)$ only apart from an irrelevant additive constant. Moreover, since $W(\underset{\sim}{k},\tau,\sigma)$ is used only for evaluation of limits as $T\to\infty$ of integrals over τ and σ of the integrands involving $W(\underset{\sim}{k},\tau,\sigma)$, it is sufficient to seek $\underset{\sim}{r}(t)$ apart from additive transient terms which occur at the boundaries $t=0$ and $t=T$ and which have finite characteristic decay times independent of T. It is also sufficient to simplify the result by retaining terms up through first order in λ only and by taking the limit $T\to\infty$.

A method of approach which seems to be fairly optimal with respect to ease and rigor is the following Fourier series technique. Any (convergent) Fourier series representation of the form

$$\bar{\underset{\sim}{r}}(t) = \left(\frac{2}{T}\right)^{\frac{1}{2}} \sum_{n=1}^{\infty} \underset{\sim}{a}(n)\ \sin(\omega_n t), \tag{D7}$$

where

$$\underset{\sim}{a}_n(t) = \left(\frac{2}{T}\right)^{\frac{1}{2}} \int_0^T dt\ \bar{\underset{\sim}{r}}(t)\ \sin(\omega_n t) \tag{D8}$$

and

$$\omega_n = n\pi/T \tag{D9}$$

will satisfy the boundary condition $\underset{\sim}{r}(o) = \underset{\sim}{r}(T) = \underset{\sim}{0}$. Similarly, since $0 < \tau < T$ and $0 < \sigma < T$,

$$\underset{\sim}{f}(\underset{\sim}{k},t,\tau,\sigma) = \left(\frac{2}{T}\right)^{\frac{1}{2}} \sum_{n=0}^{\infty} \underset{\sim}{b}(n) \sin(\omega_n t), \tag{D10}$$

where

$$\underset{\sim}{b}(n) = \left(\frac{2}{T}\right)^{\frac{1}{2}} \int_o^T dt\, \underset{\sim}{f}(t) \sin(\omega_n t). \tag{D11}$$

Insertion of Eqs. (D7) and (D10) into Eqs. (D1)-(D3), performance of the resultant integrations, neglect of transient terms proportional to e^{-wt} and $e^{-w(T-t)}$, and use of linear independence of the Fourier expansion functions, $\sqrt{(2/T)} \sin(\omega_n t)$, yield

$$a_x(n) = \frac{\omega_n^2\, g(\omega_n) b_x(n) + \lambda\omega_n\, b_y(n)}{\omega_n^4 g^2(\omega_n) + \lambda^2\, \omega_n^2}, \tag{D12}$$

$$a_y(n) = \frac{\omega_n^2\, g(\omega_n) b_y(n) - \lambda\omega_n\, b_x(n)}{\omega_n^4 g^2(\omega_n) + \lambda^2\, \omega_n^2}, \tag{D13}$$

and

$$a_z(n) = \frac{b_z(n)}{\omega_n^2 g(\omega_n)} , \tag{D14}$$

where

$$g(\omega_n) = \frac{\omega_n^2 + v^2}{\omega_n^2 + w^2} , \tag{D15}$$

wherein

$$v^2 = w^2 + \frac{4C}{w} . \tag{D16}$$

Substitution of Eqs. (D12)-(D14) into Eq. (D7), use of Eq. (D11), and use of the fact that (in view of Eq. (D9)) for an even function, $F(\omega_n)$,

$$\lim_{T\to\infty} \frac{1}{T} \sum_{n=1}^{\infty} F(\omega_n) = \lim_{T\to\infty} \frac{1}{2T} \sum_{n=-\infty}^{\infty} F(\omega_n) \tag{D17}$$

$$= \lim_{T\to\infty} \frac{1}{2T} \frac{T}{\pi} \left[\int_{-\infty}^{-\pi/T} + \int_{\pi/T}^{\infty} \right] F(\xi)\, d\xi \tag{D18}$$

$$= \frac{1}{2\pi} \, PP \int_{-\infty}^{\infty} F(\xi)\, d\xi \tag{D19}$$

lead to

$$\bar{x}(t) = \int_0^T dt' \; G_{xx}(|t-t'|) \; f_x(\underset{\sim}{k}, t', \tau, \sigma) + \int_0^T dt' \; G_{xy}(t, t') \; f_y(\underset{\sim}{k}, t', \tau, \sigma) , \tag{D20}$$

$$\bar{y}(t) = \int_0^T dt'\ G_{yx}(t,t')\ f_x(\underset{\sim}{k},t',\tau,\sigma)$$

$$+ \int_0^T dt'\ G_{yy}(|t-t'|)\ f_y(\underset{\sim}{k},t',\tau,\sigma), \tag{D21}$$

and

$$\bar{z}(t) = \int_0^T dt'\ G_{zz}(|t-t'|)\ f_z(\underset{\sim}{k},t',\tau,\sigma), \tag{D22}$$

where

$$G_{xx}(|t-t'|) = G_{yy}(|t-t'|) \tag{D23}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\xi \frac{\xi^2 g(\xi)}{\xi^4 g^2(\xi)+\lambda^2\xi^2} \left[e^{i\xi|t-t'|}-1\right], \tag{D24}$$

$$G_{xy}(t,t') = -G_{yx}(t,t') \tag{D25}$$

$$= \frac{2}{T} \sum_{n=1}^{\infty} \frac{\lambda\omega_n}{\omega_n^4 g^2(\omega_n)+\lambda^2\omega_n^2} \sin(\omega_n t)\sin(\omega_n t'), \tag{D26}$$

and

$$G_{zz}(|t-t'|) = \frac{1}{2\pi}\, PP\int_{-\infty}^{\infty} d\xi\ \frac{1}{\xi^2 g(\xi)} \left[e^{i\xi|t-t'|}-1\right]. \tag{D27}$$

In Eqs. (D20)-(D22), there have been omitted terms which are recoverable by the replacement $G(|t-t'|) \rightarrow G(|t-t'|) - G(t+t')$ everywhere a symbol $G(|t-t'|)$ occurs. Such additional terms have been neglected because they lead to additional terms in $\underset{\sim}{\bar{r}}(t)$ which are either constants or are transients occuring at t=0 with finite decay times and are therefore ignorable as previously discussed.

Equations (D20)-(D22) are of the desired form used in Chapter 3, where from Eq. (75) it may be seen that only G_{zz} and $(G_{xx}-G_{zz})$ are needed for obtaining $W(\underset{\sim}{k},\tau,\sigma)$. The evaluation of G_{zz} is straightforward and can be carried out by the method of residues as follows: Use of Eq. (D15) in Eq. (D27) gives

$$G_{zz}(|t-t'|) = \frac{1}{2\pi} PP \int_0^\infty d\xi \, \frac{\xi^2+w^2}{\xi^2(\xi^2+v^2)} \left[e^{i\xi|t-t'|}-1\right] \tag{D28}$$

$$= i\left[\frac{1}{2} (\text{Residue at } \xi=0) + (\text{Residue at } \xi=iv)\right] \tag{D29}$$

$$= -\frac{1}{2v^2}\left[\frac{v^2-w^2}{v}\left(1-e^{-v|t-t'|}\right)+w^2|t-t'|\right]. \tag{D30}$$

Equations (D24), and (D27) may be combined to obtain

$$G_{xx}-G_{zz} = -\frac{\lambda^2}{2\pi}\int d\xi\ \frac{e^{i\xi|t-t'|}-1}{\xi^2\, g^3(\xi)\,(\xi^2+\lambda^2/g^2(\xi))}\ . \qquad \text{(D31)}$$

The method of residues can again be used to evaluate the integral in Eq. (D31). With the aid of Eq. (D15) one obtains

$$G_{xx}-G_{zz} = -\lambda^2 i\ [\tfrac{1}{2}\ (\text{Residue at } \xi=0)$$

$$+\ (\text{Residue at } \xi = \frac{i\lambda}{g(0)})$$

$$+\ (\text{Residue at all other points})] \qquad \text{(D32)}$$

$$= \frac{1}{2}\frac{w^2}{v^2}\,|t-t'| + \frac{1}{2\lambda}\,[\exp\{-\frac{\lambda w^2}{v^2}\,|t-t'|\}-1]$$

$$-\ \lambda^2 i\ [\text{Residue at all other points}] \qquad \text{(D33)}$$

$$= \frac{1}{4}\,\lambda\,\frac{w^4(|t-t'|)^2}{v^4} + O(\lambda^2). \qquad \text{(D34)}$$

APPENDIX E

WEAK AND STRONG COUPLING EXPANSIONS

It is the purpose of this appendix to obtain the polaron self-energy, $E_o(\alpha)$, and effective mass, $\mu'(\alpha)$ as power series in the polaron coupling constant, α, both for $\alpha \to 0$ and for $\alpha \to \infty$. In recapitulation,

$$E_F(\alpha) = \frac{3}{4}\frac{(v-w)^2}{v} - \frac{\alpha}{\sqrt{\pi}}\frac{v}{w}\int_o^\infty du\ \frac{e^{-u}}{[J(u)]^{\frac{1}{2}}}\ , \tag{E1}$$

and

$$\mu'(\alpha) = [1-(1-\frac{w^2}{v^2})^2 - \frac{\alpha}{3\sqrt{\pi}}\frac{w}{v}\int_o^\infty du\ \frac{u^2e^{-u}}{[J(u)]^{3/2}}]^{-1}, \tag{E2}$$

where

$$J(u) = u + \frac{v^2-w^2}{vw^2}(1 - e^{-vu}), \tag{E3}$$

$$v \equiv (w^2 + \frac{4C}{w})^{\frac{1}{2}}\ , \tag{E4}$$

and C and w are variational parameters to be determined by minimizing $E_F(\alpha)$. These parameters were first introduced to approximate (apart from an additive constant)

$$S = \int_o^T dt\ (-\frac{1}{2}\dot{\underset{\sim}{r}}^2 + i\lambda\dot{x}y) + \frac{\alpha}{\sqrt{8}}\int_o^T\int_o^T dt\ ds\ \frac{e^{-|t-s|}}{|\underset{\sim}{r}(t)-\underset{\sim}{r}(s)|} \tag{E5}$$

by

$$S' = \int_0^T dt \left(-\frac{1}{2}\dot{\underset{\sim}{r}}^2 + i\lambda\dot{x}y \right)$$

$$- \frac{1}{2} C \int_0^T \int_0^T dt\, ds\, e^{-w|t-s|} [\underset{\sim}{r}(t) - \underset{\sim}{r}(s)]^2 \,. \qquad \text{(E6)}$$

Weak Coupling ($\alpha \to 0$)

A comparison of Eqs. (E5) and (E6) suggests that for small α, w be considered zeroth-order in α, and that C be taken as first order in α as an assumed starting point. Then, by use of Eq. (E4)

$$v = (1 + \eta\alpha + O(\alpha^2))w \,, \qquad \text{(E7)}$$

where η is zeroth order in α.

Using Eq. (E7), one can expand the integrand of Eq. (E1) as a power series in α and then integrate term by term to get

$$\int_0^\infty du \, \frac{e^{-u}}{[J(u)]^{\frac{1}{2}}} = \frac{\sqrt{\pi}}{w} \left\{ 1 - \frac{\eta\alpha[(w+1)^{\frac{1}{2}} - 1]}{2w} \right\} + O(\alpha^2) \,. \qquad \text{(E8)}$$

Substituting Eq. (E8) into Eq. (E1) and again using Eq. (E7) to express the rest of Eq. (E1) as a series in orders of α, one obtains an expression which has to be minimized with respect to w and η. The outcome, which confirms the initial assumptions concerning the α-dependency of v, w,

and η, is

$$\eta = (2/27) + O(\alpha^1), \tag{E9}$$

$$w = 3 + O(\alpha^1), \tag{E10}$$

$$v = 3 + (2/9)\alpha + O(\alpha^2), \tag{E11}$$

and

$$E(\alpha) = -\alpha - (1/81)\alpha^2 + O(\alpha^3). \tag{E12}$$

By substituting Eq. (E3) into Eq. (E2), using Eqs. (E10) and (E11), expanding the resultant integrand as a power series in α, and integrating term by term, one obtains

$$\mu'(\alpha) = 1 + (1/6)\alpha + (73/2916)\alpha^2 + O(\alpha^3) \tag{E13}$$

$$= 1 + .166667\alpha + .025034\alpha^2 + O(\alpha^3). \tag{E14}$$

Strong Coupling ($\alpha \to \infty$)

For the case of large α, a comparison of Eqs. (E5) and (E6) suggests that w be assumed to be zeroth order in α and C (and therefore, by Eq. (E4), also v) be assumed to go to infinity as α goes to infinity.

The integrand of Eq. (E1) can be expressed as an infinite sum of terms, in each of which the v-dependence has the form of a power of $\sqrt{v}$ multiplied by a power of quantity, $(1-e^{-vu})^{\frac{1}{2}}$. Expanding the letter factor as a power series in e^{-vu}, one obtains an integral which is easy to evaluate term by term. The result is

$$\int_0^\infty du \frac{e^{-u}}{[J(u)]^{\frac{1}{2}}} = \frac{1}{\sqrt{v}} + \frac{2\ln 2-(\frac{1}{2})w^2}{\sqrt{v^3}} + O(\frac{1}{\sqrt{v^5}}). \qquad \text{(E15)}$$

It is found that employing this result in Eq. (E1) is sufficient for applying the variational principle to determine w to a leading order in α. The outcome, in which the initial assumptions concerning the α-dependency of w and v are confirmed, is

$$w = 1 + O(\alpha^{-2}), \qquad \text{(E16)}$$

$$v = (4/9\pi)\alpha^4 - (4\ln 2-1) + O(\alpha^{-2}), \qquad \text{(E17)}$$

and

$$E(\alpha) = -\frac{\alpha^2}{3\pi} - (3\ln 2 + \frac{3}{4}) + O(\alpha^{-2}). \qquad \text{(E18)}$$

By substituting Eq. (E3) into Eq. (E2), using Eqs. (E16) and (E17), the resultant expression can be evaluated

by the same technique as was used here to evaluate (E15). The result is

$$\mu'(\alpha) = (16\alpha^4/81\pi^2) + O(\alpha^2). \qquad \text{(E19)}$$

APPENDIX F

NUMERICAL CALCULATIONS

It was pointed out in Chapter 4 that the integrations involved in the expressions for Feynman's self-energy (E_F), the present effective mass ($\mu'(\alpha)$), and Feynman's effective mass ($m_F(\alpha)$), as given by Eqs. (83)-(85) can be performed analytically only in the limiting cases of small and large values of the polaron coupling constant, α. For intermediate values of the coupling constant, E_F, $\mu'(\alpha)$, and $m_F(\alpha)$ were evaluated numerically using the Louisiana State University Computer Research Center IBM 360/65 computer. This machine employs approximately sixteen decimal digits of accuracy in the double precision mode, which was used for all numerical calculations.

For the purpose of performing the two single integrals (one in the expression for E_F and the other in the expressions for $\mu'(\alpha)$ and $m_F(\alpha)$), the trapezoidal Romberg quadrature method as programmed in the IBM Scientific Subroutine Package was modified to obtain an accuracy to within a specifiable relative error rather than absolute error. This subroutine adjusts the integration grid automatically and in such a way that each refinement samples the integrand at points evenly distributed over the integration range. With each grid refinement the

difference between the present and immediately preceeding approximation to the integral is calculated. If this difference does not decrease with successive refinements, then the integration is terminated and a "round off" error message is generated to indicate the possibility that the integration was not done to the precision necessary to obtain the integral to the required accuracy.

The upper limit used for the (improper) integrals was obtained by requiring that an analytical overestimate to the contribution from the upper limit to infinity be less than a specified fraction (5×10^{-17}) of the already accumulated contribution.

The integrals were performed to within a maximum fractional error of 5×10^{-15}. This high accuracy in the value of E_F was needed to obtain the optimizing values of the variational parameters v and w to eight significant digits of accuracy, while such an accuracy in the values of v and w was necessary to compute the percentage difference between μ' and m_F accurately to two digits after the decimal. The resulting v and w values differ by about two figures in the third significant digit from the corresponding values reported by Schultz.[20]

For a given α, the energy-minimizing values of v and w, correct to eight decimal places were obtained by the following method:

(1) The values of v and w correct to four significant digits were taken from the work of Marshall and

Mills.[26]

(2) For the given w, the self-energy (E_F) was calculated for three values of v, v (given) and v(given)$\pm\Delta v$, Δv being chosen so that the value of v is changed by one in its last significant digit. The minimum of the E_F vs. v curve for w (given) was located by a parabolic fit.

(3) Step (2) was repeated for values of w differing from the w (given) by $\pm\Delta w$, Δw having the same significance as Δv.

(4) The outcome of Step (2) and (3) gave three energy minima , one for each of the three values of w in Step (3). The minimum of these minima was also located by the parabolic-fit method. The result for E_F was called 'Best Self-Energy', $E_{v,w}$, and the result for w was called 'Best w'.

(5) Steps (2), (3), and (4) were repeated with the roles of v and w interchanged. The outcome was called, 'Best Self-energy' E_{wv} and 'Best v'.

(6) It was verified that v (given) and w (given) were accurate to within the error limits Δv and Δw.

This verification was based on three methods of checking. First, the values of 'Best v', and 'Best w' were within the corresponding error limits, Δv and Δw. Second, the self-energy at v (given) and w (given) was less than its value at the eight surrounding points, where the self-energy was calculated. Third, the difference between $E_{v,w}$ and $E_{w,v}$ was less than the typical amount by which E_F differed from point to point at the eight surrounding points. (If these results had not been verified, Step (1) would have been reinitiated with increased values of Δv and Δw).

(7) The program was reinitiated where 'Best v' and 'Best w' were used as input to replace v (given) and w (given) and Δv and Δw were reduced.

(8) Steps (1)-(7) were repeated until the output 'Best v' and 'Best w' agreed with the input v and w to eight significant figures.

In the following pages a photographically reduced copy of the computer program may be found along with the input data and the resultant output for the final run.

```
    $JOB            WATFOR,TIME=600
 1       IMPLICIT REAL*8(A-H,O-Z)
 2       DIMENSION NALPHA(7),VINPUT(7),DELV(7),WINPUT(7),DELOM(7),DELFM(7),
        1   VBEST(7),SENVB(7),SENWB(7),WBEST(7),
        2   VV(3,7),WW(3,7),VOPT(3,7),WOPT(3,7),SENV(3,7),SENW(3,7),
        3   SELFEN(3,3,7),OURMAS(3,3,7),FYNMAS(3,3,7)
 3       COMMON V,GAMMA,RELERR
 4       DATA VINPUT/3.1096198D0,3.4212945D0,4.0343437D0,5.8098890D0,
        1   9.8502496D0,1.5413235SD1,3.0082241GD1/,
        2   WINPUT/2.8706654D0,2.5603024D0,2.1400182D0,1.6036524D0,
        3   1.2822986D0,1.1620941D0,1.0762855D0/,
        4   PI/3.1415926535E9793D0/
 5       RELERR=5.D-15
 6       RTPI=DSQRT(PI)
 7       WRITE(6,1)
 8     1 FORMAT(1H1,55X,'INTEGRATION PROGRESS REPORT'///22X,'ALPHA',5X,
        1   'XUP',12X,'AREA1',21X,'AREA2',13X,'NSTEP',2X,'IER1',2X,'IER2')
 9       DO 14 K=1,7
10       IF(K.EQ.1)NALPHA(1)=1
11       IF(K.GT.1)NALPHA(K)=NALPHA(K-1)+2
12       IF(K.EQ.7)NALPHA(7)=15
13       ALPHA=NALPHA(K)
14       DELW=5.D-6
15       DELV(K)=5.D-6
16       IF(K.GE.6)DELV(K)=5.D-5
17       IERT1=0
18       IERT2=0
19       DO 13 J=1,3
20       WW(J,K)=WINPUT(K)
21       IF(J.EQ.1)WW(J,K)=WW(J,K)-DELW
22       IF(J.EQ.3)WW(J,K)=WW(J,K)+DELW
23       W=WW(J,K)
24       DO 12 I=1,3
25       VV(I,K)=VINPUT(K)
26       IF(I.EQ.1)VV(I,K)=VV(I,K)-DELV(K)
27       IF(I.EQ.3)VV(I,K)=VV(I,K)+DELV(K)
28       V=VV(I,K)
29       W2=W*W
30       V2=V*V
31       VMW=V-W
32       V2MW2=V2-W2
33       V2OW2=V2/W2
34       GAMMA=V2MW2/W2
35       C=2.DO*ALPHA*V/(W*RTPI)
36       AREA1=0.DO
37       AREA2=0.DO
38       XL=0.DO
39       XU=.5DO
40     5 CALL DPQADR(XL,XU,AREA1,AREA2,NSTEP,IER1,IER2,ERR1,ERR2)
41       IERT1=IERT1+IER1
42       IERT2=IERT2+IER2
43       IF(I.NE.2.OR.J.NE.2)GO TO 7
44       IF(K.EQ.5.AND.XL.EQ.0.)WRITE(6,1)
45       IF(XL.EQ.0.DO)WRITE(6,4)NALPHA(K),XU,AREA1,AREA2,NSTEP,IER1,IER2
46       IF(XL.NE.0.DO)WRITE(6,6)XU,AREA1,AREA2,NSTEP,IER1,IER2
47     4 FORMAT(/23X,I2,6X,F4.1,2(4X,1PD22.15),3X,I5,2(1X,I5))
48     6 FORMAT(3(1X,F4.1,2(4X,1PD22.15),3X,I5,2(1X,I5))
49     7 IF(ERR1/AREA1.LT.5.D-17.AND.ERR2/AREA2.LT.5.D-17)GO TO 8
50       XL=XU
51       XU=XU+.5DO
```

```
      GO TO 5
    8 SELFEN(I,J,K)=.75D0*VMW*VMW/V-C*AREA1
      OURMAS(I,J,K)=1.D0/(1.D0-V2MW2*V2MW2/(V2*V2)-C*AREA2/(3.D0*V20W2))
   12 FYNMAS(I,J,K)=1.D0+C*V20W2*AREA2/3.D0
      CALL OPT(VV(1,K),VV(2,K),VV(3,K),SELFEN(1,J,K),SELFEN(2,J,K),
     1   SELFEN(3,J,K),VOPT(J,K),SENW(J,K))
   13 CONTINUE
      DO 14 I=1,3
      CALL OPT(WW(1,K),WW(2,K),WW(3,K),SELFEN(I,1,K),SELFEN(I,2,K),
     1   SELFEN(I,3,K),WOPT(I,K),SENV(I,K))
   14 CONTINUE
      IF(IERT1.EQ.0.AND.IERT2.EQ.0)WRITE(6,9)
      IF(IERT1.NE.0.OR.IERT2.NE.0)WRITE(6,10)IERT1,IERT2
    9 FORMAT(1H0,50X,'NO INTEGRATION ERROR MESSAGES')
   10 FORMAT(1H0,41X,'INTEGRATION ERROR SUMMARY MESSAGE CODE',I6,',',I6)
      WRITE(6,15)
   15 FORMAT(1H1,56X,'DETAILED RESULTS'// 5X,24('*',4X))
      DO 17 K=1,7
      CALL OPT(VV(1,K),VV(2,K),VV(3,K),SENV(1,K),SENV(2,K),SENV(3,K),
     1   VBEST(K),SENVB(K))
      CALL OPT(WW(1,K),WW(2,K),WW(3,K),SENW(1,K),SENW(2,K),SENW(3,K),
     1   WBEST(K),SENWB(K))
      CALL DEVIAT(SELFEN,DELEN,K)
      CALL DEVIAT(OURMAS,DELOM(K),K)
      CALL DEVIAT(FYNMAS,DELFM(K),K)
      IF(K.EQ.4.OR.K.EQ.7)WRITE(6,15)
   17 WRITE(6,18)ALPHA(K),VINPUT(K),DELV(K),WINPUT(K),DELW,
     1   SELFEN(2,2,K),DELEN,OURMAS(2,2,K),DELOM(K),FYNMAS(2,2,K),
     2   DELFM(K),((SELFEN(I,J,K),I=1,3),J=1,3),VBEST(K),WBEST(K),
     3   SENVB(K),SENWB(K)
   18 FORMAT(5X,'ALPHA=',I2/33X,'INPUT V=',1PD22.15,1X,
     1   'WITH UNCERTAINTY',D9.2/33X,'INPUT W=',D22.15,1X,
     2   'WITH UNCERTAINTY',D9.2/34X,'SELFEN=',D22.15,1X,
     3   'WITH UNCERTAINTY',D9.2/34X,'OURMAS=',D22.15,1X,
     4   'WITH UNCERTAINTY',D9.2/34X,'FYNMAS=',D22.15,1X,
     5   'WITH UNCERTAINTY',D9.2//57X,'SELF-ENERGY TABLE'//43X,'V1',22X,
     6   'V2',22X,'V3'//27X,'W1',4X,2(D22.15,2X),D22.15,' **'/
     7   27X,'W2',4X,2(D22.15,2X),D22.15,' **'/
     8   27X,'W3',4X,2(D22.15,2X),D22.15,' **'/
     9   43X,3('**',22X)/11X,'BEST V=',0PF10.7,'   BEST W=',F10.7,3X,
     A   'BEST SELF-ENERGIES=',1PD22.15,' AND ',D22.15//5X,24('*',4X))
      WRITE(6,20)
   20 FORMAT(1H1,58X,'FINAL RESULTS'///1X,'ALPHA',9X,'V',11X,'W',11X,
     1   'SELF-ENERGY',15X,'EFFECTIVE MASS',13X,
     2   39HPERCENTAGE CORRECTION TO FEYNMAN'S MASS/)
      DO 19 K=1,7
      CORF=((OURMAS(2,2,K)-FYNMAS(2,2,K))/FYNMAS(2,2,K))*100.
      UNCORF=((DELOM(K)+DELFM(K))/FYNMAS(2,2,K))*100.
   19 WRITE(6,21)OURMAS(2,2,K),ALPHA(K),VINPUT(K),WINPUT(K),
     1   SELFEN(2,2,K),CORF,UNCORF,FYNMAS(2,2,K)
   21 FORMAT(58X,1PD17.10,2X,9HOUR  MASS/2X,I2,6X,0PF10.7,3X,F9.7,4X,
     1   1PD17.10,37X,0PF10.6,3X,'WITH UNCERTAINTY',F12.9/58X,1PD17.10,
     2   2X,9HFEYNMAN'S///)
      WRITE(6,22)
   22 FORMAT(1H1)
      STOP
      END
C
C
C
```

```
      SUBROUTINE OPQADR(XL,XU,Y1,Y2,NSTEP,IER1,IER2,ERR1,ERR2)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION AUX1(40),AUX2(40)
      COMMON V,GAMMA,RELERR
      H=XU-XL
      CALL INTGRD(XL,F1L,F2L)
      CALL INTGRD(XU,F1U,F2U)
      ERR1=F1U/(2.D0*XU)
      ERR2=F2U/(2.D0*XU)
      AUX1(1)=(F1L+F1U)/2.D0
      AUX2(1)=(F2L+F2U)/2.D0
      HH=H
      DELB1=0.D0
      DELB2=0.D0
      IER1=0
      IER2=0
      P=1.D0
      JJ=1
      Y1OLD=Y1
      Y2OLD=Y2
      NSTEP=1
      DO 3 I=2,40
      NSTEP=NSTEP+NSTEP
      Y1=AUX1(1)
      Y2=AUX2(1)
      DELA1=DELB1
      DELA2=DELB2
      HD=HH
      HH=HH/2.D0
      P=P/2.D0
      X=XL+HH
      SM1=0.D0
      SM2=0.D0
      DO 1 J=1,JJ
      CALL INTGRD(X,F1,F2)
      SM1=SM1+F1
      SM2=SM2+F2
    1 X=X+HD
      AUX1(I)=AUX1(I-1)/2.DO+P*SM1
      AUX2(I)=AUX2(I-1)/2.D0+P*SM2
      Q=1.D0
      JI=I-1
      DO 2 J=1,JI
      II=I-J
      Q=Q+Q
      Q=Q+Q
      AUX1(II)=AUX1(II+1)+(AUX1(II+1)-AUX1(II))/(Q-1.D0)
    2 AUX2(II)=AUX2(II+1)+(AUX2(II+1)-AUX2(II))/(Q-1.D0)
      DELB1=DABS((Y1-AUX1(1))/(AUX1(1)+Y1OLD/H))
      DELB2=DABS((Y2-AUX2(1))/(AUX2(1)+Y2OLD/H))
      IF(I.LT.5)GO TO 3
      IF(DELB1.LT. RELERR.AND.DELB2.LT.RELERR)GO TO 4
      IF(DELB1.GE.DELA1)GO TO 5
    3 JJ=JJ+JJ
      IER1=1000
      IER2=1000
    4 Y1=H*AUX1(1)+Y1OLD
      Y2=H*AUX2(1)+Y2OLD
      RETURN
    5 IER1=1
```

```
      IF(DELB2.GE.DELA2)IER2=1
      Y1=H*Y1+Y1OLD
      Y2=H*Y2+Y2OLD
      RETURN
      END
C
      SUBROUTINE INTGRD(XX,F1,F2)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON V,GAMMA,RELERR
      IF(XX.NE.0.D0)GO TO 5
      F1=1.D0/DSQRT(1.D0+GAMMA)
      F2=0.D0
      RETURN
    5 X2=XX*XX
      X=V*X2
      IF(X.GT.47.D0)GO TO 2
      IF(X.GT..2D0)GO TO 3
      G=1.D0
      T=1.D0
      XN=1.D0
    1 XN=XN+1.D0
      T=-X*T/XN
      OLDG=G
      G=G+T
      IF(G-OLDG)1,4,1
    2 G=1.D0/X
      GO TO 4
    3 G=(1.D0-DEXP(-X))/X
    4 F2=1.D0+G*GAMMA
      F1=DEXP(-X2)/DSQRT(F2)
      F2=X2*F1/F2
      RETURN
      END
C
      SUBROUTINE OPT(X1,X2,X3,F1,F2,F3,XOPT,FOPT)
      IMPLICIT REAL*8(A-H,O-Z)
      D12=(F1-F2)/(X1-X2)
      D23=(F2-F3)/(X2-X3)
      XOPT=((X2+X3)*D12-(X1+X2)*D23)/(2.D0*(D12-D23))
      FOPT=(F1+F2+F3-(D12-D23)*(3.D0*XOPT*XOPT+X1*X1+X2*X2+X3*X3
     1   -2.D0*XOPT*(X1+X2+X3)))/(X1-X3))/3.D0
      RETURN
      END
C
      SUBROUTINE DEVIAT(ARRAY,DELTA,K)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION ARRAY(3,3,7)
      DELTA=0.D0
      DO 1 J=1,3
      DO 1 I=1,3
      DIFF=DABS(ARRAY(I,J,K)-ARRAY(2,2,K))
      IF(DIFF.GT.DELTA)DELTA=DIFF
    1 CONTINUE
      RETURN
      END

$ENTRY
```

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ALPHA	XUP	AREA1	AREA2	NSTEP	IER1	IER2
1	0.5	4.292107695485165D-01	2.952207080925372D-02	128	0	0
	1.0	7.030238242277314D-01	1.663389219117279D-01	128	0	0
	1.5	8.102951517963048D-01	3.173364930477867D-01	64	0	0
	2.0	8.359322321928203D-01	3.889045471172300D-01	64	0	0
	2.5	8.396945719104546D-01	4.063876526838945D-01	64	0	0
	3.0	8.400342913879432D-01	4.087578951933854D-01	64	0	0
	3.5	8.400531563841102D-01	4.089425239480637D-01	64	0	0
	4.0	8.400537999055534D-01	4.089509416204271D-01	32	0	0
	4.5	8.400538133722677D-01	4.089511686998032D-01	32	0	0
	5.0	8.400538135449242D-01	4.089511723488745D-01	32	0	0
	5.5	8.400538135462787D-01	4.089511723839588D-01	16	0	0
	6.0	8.400538135462853D-01	4.089511723841612D-01	16	0	0
	6.5	8.400538135462853D-01	4.089511723841619D-01	16	0	0
3	0.5	3.544880377215805D-01	1.742802652191889D-02	128	0	0
	1.0	5.982414390531058D-01	1.168563600484630D-01	128	0	0
	1.5	6.996666741421940D-01	2.455190607389361D-01	64	0	0
	2.0	7.245527651313070D-01	3.111201581140289D-01	64	0	0
	2.5	7.282473491738458D-01	3.276876506099337D-01	64	0	0
	3.0	7.285829455389957D-01	3.299733097496126D-01	64	0	0
	3.5	7.286016461767874D-01	3.301531790942564D-01	64	0	0
	4.0	7.286022854848138D-01	3.301614330604688D-01	32	0	0
	4.5	7.286022988829219D-01	3.301616566949525D-01	32	0	0
	5.0	7.286022990548752D-01	3.301616602996846D-01	32	0	0
	5.5	7.286022990562253D-01	3.301616603344201D-01	16	0	0
	6.0	7.286022990562317D-01	3.301616603346208D-01	16	0	0
	6.5	7.286022990562317D-01	3.301616603346215D-01	16	0	0
5	0.5	2.579094348202143D-01	7.174641405401284D-03	128	0	0
	1.0	4.560727417797231D-01	6.344885885953979D-02	128	0	0
	1.5	5.469333289661140-01	1.574075068578244D-01	128	0	0
	2.0	5.703069257127022D-01	2.120035161980350D-01	64	0	0
	2.5	5.738575482168662D-01	2.267321784338112D-01	64	0	0
	3.0	5.741841320945047D-01	2.288399821422077D-01	64	0	0
	3.5	5.742024674253928D-01	2.290095668483874D-01	64	0	0
	4.0	5.742030972687481D-01	2.290174608351172D-01	32	0	0
	4.5	5.742031105116412D-01	2.290176768046459D-01	32	0	0
	5.0	5.742031106819951D-01	2.290176803098974D-01	32	0	0
	5.5	5.742031106833349D-01	2.290176803438454D-01	16	0	0
	6.0	5.742031106833413D-01	2.290176803440424D-01	16	0	0
	6.5	5.742031106833413D-01	2.290176803440430D-01	16	0	0
7	0.5	1.406238083894314D-01	1.310623782207700D-03	128	0	0
	1.0	2.706883642539103D-01	1.880651837967360D-02	128	0	0
	1.5	3.402548229855359D-01	6.237371125478264D-02	128	0	0
	2.0	3.598512011217512D-01	9.492796226760835D-02	64	0	0
	2.5	3.629959324150970-01	1.052092489051475D-01	64	0	0
	3.0	3.632952127094627D-01	1.068347488610929D-01	64	0	0
	3.5	3.633123901094477D-01	1.069743306150727D-01	64	0	0
	4.0	3.633129890379359D-01	1.069811218322184D-01	64	0	0
	4.5	3.633130017631828D-01	1.069813135065754D-01	32	0	0
	5.0	3.633130019281230D-01	1.069813166886562D-01	32	0	0
	5.5	3.633130019294275D-01	1.069813167199989D-01	32	0	0
	6.0	3.633130019294338D-01	1.069813167201831D-01	16	0	0
	6.5	3.633130019294338D-01	1.069813167201838D-01	16	0	0

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ALPHA	XUP	AREA1	AREA2	NSTEP	IER1	IER2
9	0.5	7.163399599670378D-02	2.086340212960607D-04	256	0	0
	1.0	1.530552208741693D-01	4.846649512947178D-03	256	0	0
	1.5	2.013817006572343D-01	1.987624546022027D-02	128	0	0
	2.0	2.160993377863922D-01	3.387393260685986D-02	64	0	0
	2.5	2.186155339013369D-01	3.918022988610914D-02	64	0	0
	3.0	2.188668400372905D-01	4.014634933080225D-02	64	0	0
	3.5	2.188817936661603D-01	4.023862280798107D-02	64	0	0
	4.0	2.188823293095276D-01	4.024348611196091D-02	64	0	0
	4.5	2.188823409242825D-01	4.024363194911503D-02	32	0	0
	5.0	2.188823410771935D-01	4.024363448545474D-02	32	0	0
	5.5	2.188823410784176D-01	4.024363451135715D-02	32	0	0
	6.0	2.188823410784235D-01	4.024363451151377D-02	16	0	0
	6.5	2.188823410784236D-01	4.024363451151434D-02	16	0	0
11	0.5	4.544330199131916D-02	6.467565011942616D-05	256	0	0
	1.0	1.050154025985373D-01	1.930325334727307D-03	256	0	0
	1.5	1.416416553963600-01	8.555583181347322D-03	128	0	0
	2.0	1.531887589485140D-01	1.537379285295820-02	64	0	0
	2.5	1.552325610051278D-01	1.823266008937461D-02	64	0	0
	3.0	1.554432367888022D-01	1.880369372187040D-02	64	0	0
	3.5	1.554561191498830D-01	1.886280284605319D-02	64	0	0
	4.0	1.554565912605387D-01	1.886613658865544D-02	64	0	0
	4.5	1.554566016926184D-01	1.886624233148810D-02	32	0	0
	5.0	1.554566018321043D-01	1.886624425753468D-02	32	0	0
	5.5	1.554566018332352D-01	1.886624427796717D-02	32	0	0
	6.0	1.554566018332408D-01	1.886624427809466D-02	16	0	0
	6.5	1.554566018332408D-01	1.886624427809513D-02	16	0	0
	7.0	1.554566018332408D-01	1.886624427809513D-02	16	0	0
15	0.5	2.611190678917055D-02	1.667582588063196D-05	256	0	0
	1.0	6.601496396765936D-02	5.844015727490836D-04	128	0	0
	1.5	9.107313923686560D-02	2.726154842959510-03	64	0	0
	2.0	9.918498333099817D-02	5.107790430759477D-03	64	0	0
	2.5	1.006644896323780-01	6.198267698434798D-03	64	0	0
	3.0	1.008218012970055D-01	6.436918816017346D-03	64	0	0
	3.5	1.008317152032015D-01	6.463928790454870D-03	64	0	0
	4.0	1.008320889109655D-01	6.465585103614157D-03	64	0	0
	4.5	1.008320973829322D-01	6.465641803681927D-03	32	0	0
	5.0	1.008320974988301D-01	6.465642909361168D-03	32	0	0
	5.5	1.008320974997890D-01	6.465642921819847D-03	32	0	0
	6.0	1.008320974997938D-01	6.465642921901808D-03	16	0	0
	6.5	1.008320974997938D-01	6.465642921902125D-03	16	0	0
	7.0	1.008320974997938D-01	6.465642921902125D-03	16	0	0

NO INTEGRATION ERROR MESSAGES

DETAILED RESULTS

```
*    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *
ALPHA= 1
                          INPUT V= 3.109619800000000D 00 WITH UNCERTAINTY 5.00D-06
                          INPUT W= 2.870665400000000D 00 WITH UNCERTAINTY 5.00D-06
                           SELFEN=-1.013030835360329D 00 WITH UNCERTAINTY 2.20D-11
                           OURMAS= 1.195939140483242D 00 WITH UNCERTAINTY 1.05D-06
                           FYNMAS= 1.195514700297111D 00 WITH UNCERTAINTY 1.31D-06

                                          SELF-ENERGY TABLE

                                V1                      V2                      V3

                   W1    -1.013030835360312D 00  -1.013030835354591D 00  -1.013030835338328D 00 **
                   W2    -1.013030835355096D 00  -1.013030835360329D 00  -1.013030835355021D 00 **
                   W3    -1.013030835338481D 00  -1.013030835354669D 00  -1.013030835360315D 00 **
                                **                      **                      **
      BEST V= 3.1096198   BEST W= 2.8706654   BEST SELF-ENERGIES=-1.013030835360328D 00 AND -1.013030835360329D 00

*    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *
ALPHA= 3
                          INPUT V= 3.421294500000000D 00 WITH UNCERTAINTY 5.00D-06
                          INPUT W= 2.560302400000000D 00 WITH UNCERTAINTY 5.00D-06
                           SELFEN=-3.133333544317064D 00 WITH UNCERTAINTY 1.56D-11
                           OURMAS= 1.895296249920795D 00 WITH UNCERTAINTY 5.11D-06
                           FYNMAS= 1.888953996841577D 00 WITH UNCERTAINTY 5.95D-06

                                          SELF-ENERGY TABLE

                                V1                      V2                      V3

                   W1    -3.133333544316896D 00  -3.133333544312590D 00  -3.133333544301479D 00 **
                   W2    -3.133333544313679D 00  -3.133333544317064D 00  -3.133333544313644D 00 **
                   W3    -3.133333544301555D 00  -3.133333544312631D 00  -3.133333544316903D 00 **
                                **                      **                      **
      BEST V= 3.4212945   BEST W= 2.5603024   BEST SELF-ENERGIES=-3.133333544317064D 00 AND -3.133333544317064D 00

*    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *
ALPHA= 5
                          INPUT V= 4.034343700000000D 00 WITH UNCERTAINTY 5.00D-06
                          INPUT W= 2.140018200000000D 00 WITH UNCERTAINTY 5.00D-06
                           SELFEN=-5.440144499420926D 00 WITH UNCERTAINTY 9.10D-12
                           OURMAS= 3.919759427987061D 00 WITH UNCERTAINTY 1.74D-05
                           FYNMAS= 3.885619761246900D 00 WITH UNCERTAINTY 1.90D-05

                                          SELF-ENERGY TABLE

                                V1                      V2                      V3

                   W1    -5.440144499420305D 00  -5.440144499417818D 00  -5.440144499411821D 00 **
                   W2    -5.440144499419175D 00  -5.440144499420926D 00  -5.440144499419166D 00 **
                   W3    -5.440144499411852D 00  -5.440144499417838D 00  -5.440144499420316D 00 **
                                **                      **                      **
      BEST V= 4.0343437   BEST W= 2.1400182   BEST SELF-ENERGIES=-5.440144499420923D 00 AND -5.440144499420924D 00

*    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *
```

```
                                                DETAILED RESULTS

*    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *
ALPHA= 7
                           INPUT V= 5.8C9889000000000D 00 WITH UNCERTAINTY 5.00D-06
                           INPUT W= 1.6036524000000C0D 00 WITH UNCERTAINTY 5.00D-06
                            SELFEN=-8.112687538114789D 00 WITH UNCERTAINTY 5.54D-12
                            OURMAS= 1.452979907149292D 01 WITH UNCERTAINTY 7.04D-05
                            FYNMAS= 1.439407027254799D 01 WITH UNCERTAINTY 7.77D-05

                                                SELF-ENERGY TABLE

                                  V1                       V2                       V3

                     W1    -8.112687538112435D 00  -8.112687538111584D 00  -8.112687538109314D 00 **
                     W2    -8.112687538114080D 00  -8.112687538114789D 00  -8.112687538114077D 00 **
                     W3    -8.112687538109251D 00  -8.112687538111522D 00  -8.112687538112370D 00 **
                                     **                      **                      **
      BEST V= 5.8098890   BEST W= 1.6036524   BEST SELF-ENERGIES=-8.112687538114784D 00 AND -8.112687538114784D 00

*    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *
ALPHA= 9
                           INPUT V= 9.850249600000000D 00 WITH UNCERTAINTY 5.00D-06
                           INPUT W= 1.282298600000000D 00 WITH UNCERTAINTY 5.00D-06
                            SELFEN=-1.148578624337449D 01 WITH UNCERTAINTY 8.42D-12
                            OURMAS= 6.300500630491279D 01 WITH UNCERTAINTY 2.15D-04
                            FYNMAS= 6.275152852899188D 01 WITH UNCERTAINTY 2.55D-04

                                                SELF-ENERGY TABLE

                                  V1                       V2                       V3

                     W1    -1.148578624336799D 01  -1.148578624336743D 01  -1.148578624336607D 01 **
                     W2    -1.148578624337410D 01  -1.148578624337449D 01  -1.148578624337408D 01 **
                     W3    -1.148578624336622D 01  -1.148578624336756D 01  -1.148578624336810D 01 **
                                     **                      **                      **
      BEST V= 9.8502496   BEST W= 1.2822986   BEST SELF-ENERGIES=-1.148578624337449D 01 AND -1.148578624337449D 01

*    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *
ALPHA=11
                           INPUT V= 1.541323550000000D 01 WITH UNCERTAINTY 5.00D-05
                           INPUT W= 1.162094100000000D 00 WITH UNCERTAINTY 5.00D-06
                            SELFEN=-1.570980845496904D 01 WITH UNCERTAINTY 4.52D-11
                            OURMAS= 1.834330269015660D 02 WITH UNCERTAINTY 1.35D-03
                            FYNMAS= 1.831249713863436D 02 WITH UNCERTAINTY 1.46D-03

                                                SELF-ENERGY TABLE

                                  V1                       V2                       V3

                     W1    -1.570980845493917D 01  -1.570980845495850D 01  -1.570980845492389D 01 **
                     W2    -1.570980845494209D 01  -1.570980845496904D 01  -1.570980845494205D 01 **
                     W3    -1.570980845492423D 01  -1.570980845495880D 01  -1.570980845493944D 01 **
                                     **                      **                      **
      BEST V=15.4132355   BEST W= 1.1620941   BEST SELF-ENERGIES=-1.570980845496904D 01 AND -1.570980845496904D 01

*    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *
```

DETAILED RESULTS

* *

ALPHA=15

INPUT V= 3.008224160000000D 01 WITH UNCERTAINTY 5.000D-05
INPUT W= 1.076285500000000D 00 WITH UNCERTAINTY 5.000D-06
SELFEN=-2.672490398788998D 01 WITH UNCERTAINTY 3.370D-11
OURMAS= 7.978454132332941D 02 WITH UNCERTAINTY 2.940D-03
FYNMAS= 7.974983790870424D 02 WITH UNCERTAINTY 3.230D-03

SELF-ENERGY TABLE

	V1	V2	V3	
W1	-2.672490398786614D 01	-2.672490398787591D 01	-2.672490398785635D 01	**
W2	-2.672490398787530D 01	-2.672490398788998D 01	-2.672490398787534D 01	**
W3	-2.672490398785626D 01	-2.672490398787585D 01	-2.672490398786612D 01	**
	**	**	**	

BEST V=30.0822416 BEST W= 1.0762855 BEST SELF-ENERGIES=-2.672490398788998D 01 AND -2.672490398788998D 01

* *

FINAL RESULTS

ALPHA	V	W	SELF-ENERGY	EFFECTIVE MASS	PERCENTAGE CORRECTION TO FEYNMAN'S MASS
1	3.1096198	2.8706654	-1.0130308354D 00	1.19593914050 00 OUR MASS 1.19551470030 00 FEYNMAN'S	0.035503 WITH UNCERTAINTY 0.000197011
3	3.4212945	2.5603024	-3.13333354430 00	1.89529624990 00 OUR MASS 1.88895399680 00 FEYNMAN'S	0.335755 WITH UNCERTAINTY 0.000585746
5	4.0343437	2.1400182	-5.44014449940 00	3.91975942800 00 OUR MASS 3.88561976120 00 FEYNMAN'S	0.878616 WITH UNCERTAINTY 0.000936821
7	5.8098890	1.6036524	-8.11268753810 00	1.45297990710 01 OUR MASS 1.43940702730 01 FEYNMAN'S	0.942949 WITH UNCERTAINTY 0.001028877
9	9.8502496	1.2822986	-1.14857862430 01	6.30050063050 01 OUR MASS 6.27515285290 01 FEYNMAN'S	0.403939 WITH UNCERTAINTY 0.000749169
11	15.4132355	1.1620941	-1.57098084550 01	1.83433026900 02 OUR MASS 1.83124971390 02 FEYNMAN'S	0.168221 WITH UNCERTAINTY 0.001536928
15	30.0822416	1.0762855	-2.67249039880 01	7.97845413230 02 OUR MASS 7.97498379090 02 FEYNMAN'S	0.043515 WITH UNCERTAINTY 0.000773462

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VITA

Manmohan Singh Chawla was born in Bikaner, India on July 12, 1940. In 1956 he received his high school diploma from the University of Rajasthan, setting a new scholastic record. In 1963 he received his Masters degree in Physics from Birla Institute of Science and Technology at Pilani. For the period 1956-63, he was a recipient of a Government of India Merit Scholarship. For the period 1963-64, he was a Junior Research Fellow for Council of Scientific and Industrial Research. In 1965 he earned an Associateship of the Saha Institute of Nuclear Physics of Calcutta University. In September 1965, he entered Louisiana State University at Baton Rouge as a graduate student in physics. In 1968 he was elected for membership in Pi Mu Epsilon, a mathematics honorary fraternity, and in 1970 he was elected for membership in Phi Sigma Phi, a national scholastic fraternity. He is presently a candidate for the degree of Doctor of Philosophy in the Department of Physics and Astronomy.

EXAMINATION AND THESIS REPORT

Candidate: Manmohan Singh Chawla

Major Field: Physics

Title of Thesis: A Feynman Path-Integral Calculation of the Polaron Effective Mass

Approved:

John T. Marshall
Major Professor and Chairman

Max Goodrich
Dean of the Graduate School

EXAMINING COMMITTEE:

Joseph Callaway

R. W. LeBlanc

Leonard C. Adams

John J. Matese

John L. Fry

Date of Examination:

August 5, 1970